

# QCDINS 2.0 – A Monte Carlo generator for instanton-induced processes in deep-inelastic scattering<sup>★</sup>

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## Abstract

We describe a Monte Carlo event generator for the simulation of QCD-instanton induced processes in deep-inelastic scattering (HERA). The QCDINS package is designed as an “add-on” hard process generator interfaced to the general hadronic event simulation package HERWIG. It incorporates the theoretically predicted production rate for instanton-induced events as well as the essential characteristics that have been derived theoretically for the partonic final state of instanton-induced processes: notably, the flavour democratic and isotropic production of the partonic final state, energy weight factors different for gluons and quarks, and a high average multiplicity  $\mathcal{O}(10)$  of produced partons with a Poisson distribution of the gluon multiplicity. While the subsequent perturbative evolution of the generated partons is always handled by the HERWIG package, the final hadronization step may optionally be performed also by means of the general hadronic event simulation package JETSET.

*Key words:* QCD; Instanton; Deep-inelastic scattering; Monte Carlo simulation  
*PACS:* 11.15.Kc; 12.38.Lg; 13.60.Hb

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<sup>★</sup> Information and code via WWW URL: [www.desy.de/~t00fri/qcdins/qcdins.html](http://www.desy.de/~t00fri/qcdins/qcdins.html)

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## PROGRAM SUMMARY

*Title of program:* QCDINS 2.0

*Catalogue identifier:*

*Program obtainable from:* <http://www.desy.de/~t00fri/qcdins/qcdins.html>

*Computer for which the program is designed and others on which it has been tested:*  
Any computer with a FORTRAN 77 compiler

*Operating systems under which the program has been tested:* Linux 2.0.X; HP-UX 10.2

*Programming language used:* FORTRAN 77

*Memory required to execute with typical data:* Size of executable program is approximately 2.6 MB. The size of the QCDINS library itself is about 200 KB; the required routines from the HERWIG and JETSET libraries constitute the dominant portion of the needed memory.

*No. of processors used:* 1

*Has the code been vectorised or parallelized?:* no

*No. of bytes in distributed program, including test data, etc.:* 1071106

*Distribution format:* ASCII

*CPC Program Library subprograms used:* HERWIG [1] version 5.9; JETSET 7.4 [2]

*Keywords:* QCD; Instanton; Deep-inelastic scattering; Monte Carlo simulation

### *Nature of physical problem*

Instantons are a basic aspect of Quantum Chromodynamics. Being non-perturbative fluctuations of the gauge fields, they induce hard processes absent in conventional perturbation theory. Deep-inelastic lepton-nucleon scattering at HERA offers a unique possible discovery window for such processes induced by QCD-instantons through their characteristic final-state signature and a sizable rate, calculable within instanton-perturbation theory. An experimental discovery of such a novel, non-perturbative manifestation of non-abelian gauge theories would be of fundamental significance. However, instanton-induced events are expected to make up only a small fraction of all deep-inelastic events. Therefore, a detailed knowledge of the resulting hadronic final state, along with a multi-observable analysis of experimental data by means of Monte Carlo techniques, is necessary.

### *Method of solution*

The QCDINS package is designed as an “add-on” hard process generator interfaced to the general hadronic event simulation package HERWIG. It incorporates the theoretically predicted production rate for instanton-induced events as well as the

essential characteristics that have been derived theoretically for the partonic final state of instanton-induced processes: notably, the flavour democratic and isotropic production of the partonic final state, energy weight factors different for gluons and quarks, and a high average multiplicity  $\mathcal{O}(10)$  of produced partons with a Poisson distribution of the gluon multiplicity. While the subsequent perturbative evolution of the generated partons is always handled by the HERWIG package, the final hadronization step may optionally be performed also by means of the general hadronic event simulation package JETSET.

*Restrictions on the complexity of the problem*

The default values of the implemented kinematical cuts represent the state of the art limits for the reliability of the generated instanton-induced event rate and event topology.

*Typical running time*

10 - 100 events per second for a PC with Pentium CPU, depending on its clock frequency. On a HP 9000/735 (99 MHz) workstation, 6 events per second are generated.

*Unusual features of the program*

none

*References*

- [1] G. Marchesini et al., Comput. Phys. Commun. 67 (1992) 465.
- [2] T. Sjöstrand, Comput. Phys. Commun. 82 (1994) 74.

# LONG WRITE-UP

## 1 Introduction

The ground state (“vacuum”) of non-abelian gauge theories like QCD is known to be very rich. It includes topologically non-trivial fluctuations of the gauge fields, carrying an integer topological charge  $Q$ . The simplest building blocks of topological structure in the vacuum are [1,2] *instantons* with  $Q = +1$  and *anti-instantons* with  $Q = -1$ . Instantons represent gluon field configurations that are localized (“instantaneous”) in Euclidean time and space. While they are believed to play an important role in various long-distance aspects of QCD, there are also important short-distance implications. In QCD with  $n_f$  (light) flavours, instantons induce hard processes violating *chirality* in accord [2] with the selection rule  $\Delta \textit{chirality} = 2 n_f Q$ , due to the general chiral anomaly. While in ordinary perturbative QCD ( $Q = 0$ ) these processes are forbidden, their experimental discovery would clearly be of basic significance. The deep-inelastic scattering regime is strongly favoured in this respect, since hard instanton-induced processes are both calculable [3,4] within instanton-perturbation theory and have good prospects for experimental detection at HERA [4–7].

QCDINS [6] is a Monte Carlo package for simulating QCD-instanton induced scattering processes in deep-inelastic scattering (HERA). It is designed as an “add-on” hard process generator interfaced by default to the Monte Carlo generator HERWIG [8]. It incorporates the theoretically predicted production rate for instanton-induced events as well as the essential characteristics that have been derived theoretically for the partonic final state of instanton-induced processes: notably, the flavour democratic [2] and isotropic [5,9] production of the final state partons, energy weight factors different for gluons and quarks [3], and a high average multiplicity  $2n_f + \mathcal{O}(1/\alpha_s)$  of produced partons with a (approximate) Poisson distribution of the gluon multiplicity [5,9,10].

Earlier versions of QCDINS have been used already to establish first experimental bounds on the rate of instanton-induced events at HERA [11–13] and to develop instanton search strategies [7].

In the present report a comprehensive description is given of the theoretical framework built into the program (Section 2) as well as of the various program components (Section 3) and of their usage (Section 4).

## 2 Instanton-induced events in deep-inelastic scattering

Let us briefly summarize in this section the underlying physics picture, some relevant formulae and the main stages involved in QCDINS to generate the complete instanton-induced partonic final state. The remaining formulae may be found under the corresponding descriptions of QCDINS routines in Section 3.

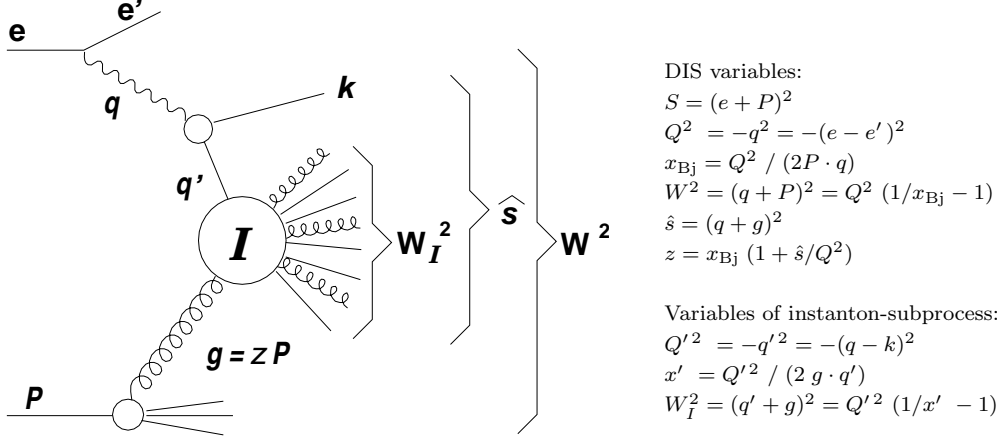


Fig. 1. Structure and kinematic variables of the dominant instanton-induced process in deep-inelastic scattering.

In deep-inelastic  $e^\pm P$  scattering, instanton-induced events are predominantly associated [4] with a process structure as sketched in Fig. 1: A photon splitting into a  $q\bar{q}$ -pair fuses with a gluon from the proton in the background of an instanton ( $I$ ) or an anti-instanton ( $\bar{I}$ ). For each (light) flavour,  $q = \{d, u, s, \dots\}$ , a violation of *chirality* is induced,

$$\Delta \text{chirality}(q) \equiv \Delta [\#(q_R + \bar{q}_R) - \#(q_L + \bar{q}_L)] = \pm 2 \quad \text{for an } \begin{cases} I \\ \bar{I} \end{cases}, \quad (1)$$

in agreement with the general chiral anomaly relation [2]. Correspondingly, the partonic final state exhibits “flavour democracy”, i. e.  $q_R \bar{q}_R$  ( $q_L \bar{q}_L$ ) pairs of *all*  $n_f$  light flavours occur precisely once in case of an instanton (anti-instanton),

$$\gamma^* + g \xrightarrow{I(\bar{I})} \sum_{q=d,u,s,\dots} [q_{R(L)} + \bar{q}_{R(L)}] + n_g g. \quad (2)$$

As illustrated in Fig. 1, one of those partons acts as a current-quark (jet)  $k$ , whereas the other  $2n_f - 1$  (anti-)quarks and some number  $n_g$  of gluons are

directly emitted from the instanton (anti-instanton) “blob”. Instanton-induced processes initiated by a quark from the proton are suppressed by a factor of  $\alpha_s^2$  with respect to the gluon initiated process [4]. This fact, together with the high gluon density in the relevant kinematical domain at HERA, justifies to neglect quark initiated processes.

In instanton-perturbation theory, the dominant instanton-induced contribution to the inclusive  $eP$  cross section<sup>3</sup>, subject to appropriate kinematical restrictions and (theoretical) fiducial cuts, has a convolution-like structure [4],

$$\begin{aligned}
\sigma_{eP}^{(I)}(\text{cuts}) &\simeq \frac{2\pi\alpha^2}{S} \sum_{q'=d,u,s,\dots;\bar{d},\bar{u},\bar{s},\dots} e_{q'}^2 \int_{Q_{\min}^{\prime 2}}^{Q_{\max}^{\prime 2}} dQ^{\prime 2} \int_{x'_{\min}}^{x'_{\max}} \frac{dx'}{x'} \frac{\sigma_{q'g}^{(I)}(x', Q^{\prime 2})}{x'} \\
&\times \int_{\max\left(\frac{Q^{\prime 2}}{Sx'y_{\text{Bj max}}}, \frac{x_{\text{Bj min}}}{x'}\right)}^{z_{\max}} \frac{dz}{z} f_g(z) \int_{x_{\text{Bj min}}}^{x'z - \frac{m_k^2}{S} \frac{1}{y_{\text{Bj max}} - \frac{Q^{\prime 2}}{Sx'z}}} \frac{dx_{\text{Bj}}}{x_{\text{Bj}}} \quad (3) \\
&\times \int_{\max\left(\frac{Q^{\prime 2}}{Sx'z} + \frac{m_k^2}{S} \frac{1}{x'z - x_{\text{Bj}}}, y_{\text{Bj min}}\right)}^{y_{\text{Bj max}}} \frac{dy_{\text{Bj}}}{y_{\text{Bj}}} \theta(Sx_{\text{Bj}}y_{\text{Bj}} - Q_{\min}^2) \\
&\times \frac{1 + (1 - y_{\text{Bj}})^2}{y_{\text{Bj}}} P_{q'}^{(I)} .
\end{aligned}$$

It involves integrations over the gluon density  $f_g(z)$ , the virtual photon flux and the flux of virtual (anti-)quarks  $q'$  in the instanton-background [4,14],

$$P_{q'}^{(I)} = \frac{3}{16\pi^3} \frac{x_{\text{Bj}}}{z x'} \left( 1 + \frac{z}{x_{\text{Bj}}} - \frac{1}{x'} - \frac{Q^{\prime 2}}{Sx_{\text{Bj}}y_{\text{Bj}}} \right) . \quad (4)$$

All relevant kinematical variables in Eq. (3) are defined in Fig. 1, and  $e_{q'}^2$  denotes the electric charge squared of the virtual (anti-)quark  $q'$  in units of the electric charge squared  $e^2 = 4\pi\alpha$ .

In Eq. (3),  $\sigma_{q'g}^{(I)}$  denotes the instanton-induced total cross section of the  $q'g$ -subprocess (c.f. Fig. 1) and contains the essential instanton dynamics. Its analytical form [4] used in QCDINS may be found in Eq. (17). As illustrated

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<sup>3</sup> A sum over instanton-induced and anti-instanton induced processes is always implied by the superscript  $(I)$  at cross sections.

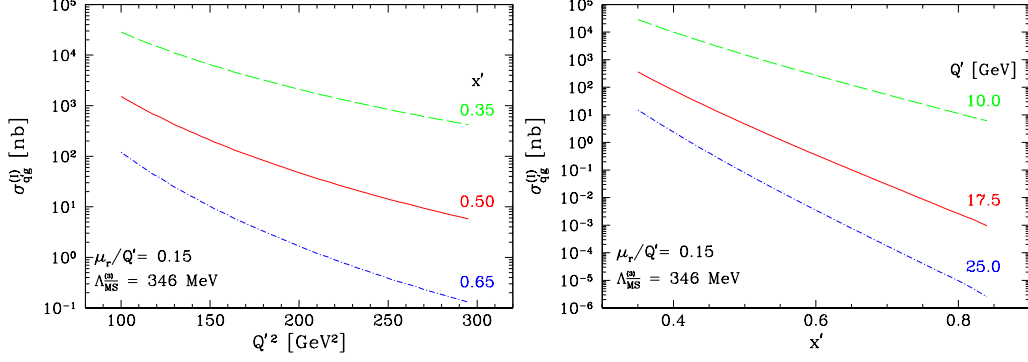


Fig. 2. Instanton-subprocess cross section (17) from Ref. [4] for  $n_f = 3$  and  $\Lambda_{\overline{\text{MS}}}^{(3)}$  from Eq. (7). It exhibits a strong dependence on the corresponding Bjorken variables  $Q'^2$  and  $x'$ , respectively.

in Fig. 2,  $\sigma_{q'g}^{(I)}$  is very steeply growing for decreasing values of  $Q'^2$  and  $x'$ , respectively. Eventually, our theoretical predictions based on instanton-perturbation theory [4] will cease to hold. Therefore, the following cuts inferred from a high-quality lattice simulation of QCD [15] are implemented by default in QCDINS 2.0 (Table 4),

$$Q' \geq Q'_{\min} = 30.8 \Lambda_{\overline{\text{MS}}}^{(n_f)}; \quad x' \geq x'_{\min} = 0.35. \quad (5)$$

A further cut on the photon virtuality,

$$Q \equiv \sqrt{Sx_{\text{Bj}}y_{\text{Bj}}} \geq Q_{\min} = Q'_{\min}, \quad (6)$$

is applied in order to warrant sufficient suppression of non-planar contributions [3], which are hard to calculate and may spoil the validity of Eq. (3).

The cross section  $\sigma_{q'g}^{(I)}$  exhibits a rather weak residual dependence on the renormalization scale  $\mu_r$ . As an “optimal” choice, the value  $\mu_r = 0.15 Q'$ , corresponding to the minimum [4],  $\partial\sigma_{q'g}/\partial\mu_r = 0$ , is taken by default (Table 4).

However,  $\sigma_{q'g}^{(I)}$  depends strongly on the QCD scale  $\Lambda_{\overline{\text{MS}}}^{(n_f)}$ . Since, strictly speaking, the underlying theoretical framework refers to massless quarks, the (default) number of flavours is set to  $n_f = 3$  (Table 4). The respective value

$$\Lambda_{\overline{\text{MS}}}^{(3)} = 0.346^{+0.031}_{-0.029} \text{ GeV}, \quad (7)$$

is obtained by a standard 3-loop perturbative flavour reduction (Eq. (9.7) of Ref. [16]) from the 1998 world-average of the running QCD coupling at the

Z-boson mass [16],

$$\alpha_s(M_Z) = 0.119 \pm 0.002 \quad \overset{3\text{-loop}}{\Leftrightarrow} \quad \Lambda_{\overline{\text{MS}}}^{(5)} = 0.219^{+0.025}_{-0.023} \text{ GeV}. \quad (8)$$

The central values of these parameters are taken as default in QCDINS 2.0 (Table 4). This upgrade of  $\Lambda_{\overline{\text{MS}}}^{(n_f)}$ , together with the modified cuts (5) and (6), represents an improved understanding of the input parameters and a considerable reduction of uncertainties, as compared to the original publication [4] and earlier versions of QCDINS. Note that it also implies a significant change in the predicted rate.

Next, let us summarize the various stages of event generation by means of QCDINS.

In a first stage, the various Bjorken variables  $Q'^2, x', z, x_{\text{Bj}}, y_{\text{Bj}}$  of the instanton-induced process (c.f. Fig. 1) are generated, with a distribution according to the normalized differential cross section from Eq. (3),

$$\frac{1}{\sigma_{eP}^{(I)}} \frac{d^5 \sigma_{eP}^{(I)}}{dQ'^2 dx' dz dx_{\text{Bj}} dy_{\text{Bj}}}. \quad (9)$$

In the second stage of the event generation, the 4-momenta  $g, q, q', k$  of the incoming gluon  $g$ , the virtual photon  $q$ , the virtual quark  $q'$  and the current quark  $k$ , respectively, are filled. Sudakov decompositions of these momenta are used to incorporate various constraints, e.g. on the momenta squared. The 4-momentum  $e'$  of the outgoing lepton is calculated subsequently.

In the third stage, the partonic final state of the instanton-induced  $q'g$ -subprocess is generated in its centre-of-mass system (CMS) as follows. The number  $n_g$  of produced gluons is generated according to a Poisson distribution with mean  $\langle n_g \rangle^{(I)}(x', Q') \sim 1/\alpha_s \sim 3$  (for the cuts (5)), as calculated theoretically (Eq. (13)) in instanton-perturbation theory [5,9,10]. Next,  $n_f (= 3)$   $[q \dots \bar{q}]$ -“strings” of partons are set up, each beginning with a quark, followed by a random number  $\leq n_g + 1$  of gluons and ending with an anti-quark of randomly chosen flavour. There are  $n_g + 1$  gluons in total and, due to the required flavour democracy (2),  $q\bar{q}$ -pairs of all  $n_f$  flavours occur precisely once. A quark and a gluon among these  $2n_f + n_g + 1$  partons are (randomly) marked as incoming.

The momenta  $p_i$  of the  $n = 2n_f - 1 + n_g$  outgoing partons are then generated in the CMS of the instanton subprocess, according to the energy-weighted phase-space



$$\begin{aligned}
& \int \prod_{i=1}^{2n_f-1} \left\{ d^4 p_i \delta^{(+)}(p_i^2 - m_i^2) p_i^0 \right\} \prod_{k=1}^{n_g} \left\{ d^4 p_k \delta^{(+)}(p_k^2 - m_g^2) p_k^{02} \right\} \\
& \times \delta^{(3)} \left( \sum_{i=1}^{2n_f-1} \vec{p}_i + \sum_{k=1}^{n_g} \vec{p}_k \right) \delta \left( W_I - \sum_{i=1}^{2n_f-1} p_i^0 - \sum_{k=1}^{n_g} p_k^0 \right).
\end{aligned} \tag{10}$$

These different energy weights for quarks and gluons [3], along with the angular isotropy [5,9], are characteristic features of the leading-order partonic final state (after averaging over colour).

Next, the colour and flavour connections of the partons are set up. The colour flow is obtained simply by connecting the colour lines of adjacent partons within each of the above-mentioned  $n_f$  [ $q \dots \bar{q}$ ]-“strings” in a planar manner (consistent with the leading order  $1/N_c$  expectation). This choice is inspired by the leading-order partonic final state (after averaging over colour) [3], but may well deserve further research. The flavour flow is constructed by connecting the flavour lines of the quark at the beginning of a string with the flavour line of the anti-quark at the end of a string.

The hard subprocess generation ends by boosting the momenta of the final state partons to the laboratory frame.

While the subsequent perturbative evolution of the generated partons is always handled by the HERWIG [8] package, the final hadronization step may optionally<sup>4</sup> be performed also by means of JETSET [18].

### 3 The QCDINS package

This section is devoted to a systematic description of the various routines of the QCDINS package that is designed as an “add-on” hard process generator, interfaced to the Monte Carlo generator HERWIG [8].

This reference section is organized as follows:

While all subroutines and functions of the QCDINS package are described in *alphabetical order* in Section 3.1, a *logical flow-chart* is provided in form of Tables 1 and 2 below. They should always be used as the main guide through the description of the package. A routine listed in the  $n$ -th column and the  $m$ -th row of these tables progressively calls all routines in the  $(n+1)$ -th column starting in the  $(m+1)$ -th row. All routines called at the level of the main hard process generator **QIHGEN** and below are documented in Table 2.

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<sup>4</sup> We thank H. Jung for his help [17] to interface QCDINS with JETSET.

Initialize input parameters (Tables 4, 5)	<b>QIINIT</b>				
Flavour reduction: $\Lambda_{\overline{\text{MS}}}^{(5)} \Rightarrow \Lambda_{\overline{\text{MS}}}^{(n_f < 5)}$		<b>LAMNF</b>			
Initialize “particle” INST in event record		<b>QIINI</b>			
Print input parameters and warnings	<b>QISTAT</b>				
Initialize JETSET common block data	<b>GJEINI</b>				
Loop over desired number of events	<b>QCLOOP</b>				
Generate one event		<b>QCDGEN</b>			
Assign hard process variables (HERWIG)			<i>HWEPRO</i>		
No action (modified HERWIG routine)				<b>HWEGAM</b>	
Call main instanton process generator				<b>HVHBVI</b>	
Main (hard) instanton process generator					<b>QIHGEN</b>
Generate parton cascades (HERWIG)			<i>HWBGEN</i>		
Combine jets with correct kinematics				<b>HWBJCO</b>	
Convert HERWIG to JETSET block data			<b>HERLUND</b>		
JETSET event record to HEPEVT common			<b>LUHEPC</b>		

Table 1

Flow-chart of QCDINS routines: A routine in the  $n$ -th column and the  $m$ -th row progressively calls all routines in the  $(n+1)$ -th column starting in the  $(m+1)$ -th row. All routines called at the level of the main hard process generator **QIHGEN** and below are listed in Table 2.

A specific application requires the writing of a steering program by the user (c.f. Section 4 and Appendix A). It must contain the standard HERWIG-initialization calls as well as the calls to various initialization routines for QCDINS. The latter comprise essentially the four routines listed in the second column of Table 1. By calling the last one of these (**QCLOOP**), the user starts the proper simulation which comprises the chain of internally called QCDINS routines as documented in Tables 1 and 2. A specific and quite extensive example is provided with the QCDINS distribution (`'qtesthz.F'`) and may be found in the directory `'qcdtest'`. It also illustrates the use of the event analysis routine **HWANAL** called by HERWIG after each processed event.

Optional account of initial state radiation from lepton	<b>EXFRAC</b>		
Check kinematical boundaries	<b>QICALC</b>		
Generate identity code of current quark $k$ and virtual quark $q'$	<b>QIHPAR</b>		
Generate $(Q', x')$ and associated weight	<b>QIHINS</b>		
Generate $X = Q'^2, x'$ as $dX/X^{(N+1)}$		<b>QIRDIS</b>	
Calculate total cross section of instanton-induced subprocess $q'g \xrightarrow{(I)} X$		<b>Q2SIG</b>	
Calculate $\bar{I}\bar{I}$ -valley action $S^{(\bar{I}\bar{I})}(\xi)$			<b>ACTION</b>
Calculate fermionic overlap $\omega(\xi)$			<b>OMEGA</b>
Calculate Lambert W-function			<b>LAMBERTW</b>
Calculate saddle-point value of conformally invariant $\bar{I}\bar{I}$ -distance $\xi$			<b>XI</b>
Calculate inverse running coupling $\frac{4\pi}{\alpha_{\overline{\text{MS}}}}$			<b>XQS</b>
Generate number $n_g$ of emitted gluons	<b>QIGMUL</b>		
Calculate gluon multiplicity $\langle n_g \rangle^{(I)}$		<b>GMULT</b>	
Calculate inverse running coupling $\frac{4\pi}{\alpha_{\overline{\text{MS}}}}$			<b>XQS</b>
Calculate $\bar{I}\bar{I}$ -valley action $S^{(\bar{I}\bar{I})}(\xi)$			<b>ACTION</b>
Calculate Lambert W-function			<b>LAMBERTW</b>
Calculate flux of virtual quark $q'$	<b>QISPLT</b>		
Calculate remaining weight	<b>QIPVWT</b>		
Calculate momentum of incoming gluon	<b>QIKPAR</b>		
Generate momentum of virtual photon	<b>QIKGAM</b>		
Generate momenta of virtual quark $q'$ and current quark $k$	<b>QIKGSP</b>		
Generate partonic final state	<b>QISTID</b>		
Generate the partons of the instanton subprocess in form of $[q \dots \bar{q}]$ -”strings”		<b>QIGLST</b>	
Find the incoming partons in the $[q \dots \bar{q}]$ -strings		<b>QIGPAR</b>	
Assign masses of outgoing partons		<b>QIPLST</b>	
Generate 4-momenta of outgoing partons		<b>QIPSGN</b>	
Calculate relative energy weight of outgoing partons			<b>QIPSWT</b>
Store 4-momenta of outgoing partons into PHEP common block of HERWIG		<b>QIPSTO</b>	
Colour/flavour connections for each string		<b>QICCON</b>	

Table 2

All routines called at the level of the main hard process generator **QIHGEN** and below. As in Table 1, a routine in the n-th column and the m-th row progressively calls all routines in the (n+1)-th column starting in the (m+1)-th row. The displayed sequence of calls corresponds to the default settings of control flags.

### 3.1 Subroutines and functions

#### SUBROUTINE **ACTION** (XI4, S, DS, DDS)

*Purpose:* Calculation of the  $I\bar{I}$ -action as well as its 1st and 2nd derivatives, as function of the conformally invariant  $I\bar{I}$ -distance.

*Arguments:*

XI4: conformally invariant  $I\bar{I}$ -distance  $\xi$ .

S:  $I\bar{I}$ -action  $S^{(I\bar{I})}(\xi)$ , Eq. (11).

DS:  $dS^{(I\bar{I})}/d\xi$ ,

DDS:  $d^2 S^{(I\bar{I})}/d\xi^2$

*Procedure:*

The action is calculated according to the exact valley form [19,20],

$$S^{(I\bar{I})}(\xi) = 1 - \frac{12}{f(\xi)} - \frac{96}{f(\xi)^2} + \frac{48}{f(\xi)^3} [3f(\xi) + 8] \ln \left[ \frac{1}{2\xi} (f(\xi) + 4) \right], \quad (11)$$

$$f(\xi) = \xi^2 + \sqrt{\xi^2 - 4}\xi - 4. \quad (12)$$

#### SUBROUTINE **EXFRAC** (A)

*Purpose:* Optional account of initial state radiation from the lepton.

*Arguments:*

A: = 1.0; dummy rescaling factor of the incoming lepton momentum; double precision output variable.

*Remarks:* The actual routine has to be provided by the user.

#### SUBROUTINE **GJEINI**

*Purpose:* Initialization of the JETSET [18] parameter common blocks LUDAT1, LUDAT2, LUDAT3, LUDAT4 and LUDATR.

*Remarks:* **GJEINI** has to be called by the user before any other JETSET routine. **GJEINI** is from Ref. [21].

## FUNCTION

**GMULT** (XPR, XL\_MIN, XL\_MAX, QLAM, KAPPA, NF, LOOPFL)

*Purpose:* Calculation of the average gluon multiplicity  $\langle n_g \rangle^{(I)}$  depending on  $x'$ ,  $Q'/\Lambda_{\overline{\text{MS}}}^{(n_f)}$ ,  $\mu_r/Q'$ ,  $n_f$  and loop-order. Here,  $\mu_r$  and  $n_f$  denote the renormalization scale and the number of light flavours, respectively.

*Arguments:*

XPRIME:  $x'$

XL\_MIN:  $\xi_{\min}$ ; lower boundary of  $\xi$  used for interpolation.

XL\_MAX:  $\xi_{\max}$ ; upper boundary of  $\xi$  used for interpolation.

QLAM:  $Q'/\Lambda_{\overline{\text{MS}}}^{(n_f)}$

KAPPA:  $\mu_r/Q'$

NF:  $n_f$ ; number of light flavours.

LOOPFL: = 1: 1-loop renormalization group (RG) invariance [4] along with 1-loop form of  $\alpha_s$ .

= 2: 2-loop RG invariance [4] along with 2-loop form of  $\alpha_{\overline{\text{MS}}}$ .

= 3: (default) 2-loop RG invariance along with 3-loop form of  $\alpha_{\overline{\text{MS}}}$ .

*Procedure:*

From an analysis based on the generalized (Mueller [22]) optical theorem for the  $q'g\bar{g}$  forward scattering amplitude and the  $I\bar{I}$ -valley method, one infers [9] the differential one-gluon inclusive  $q'g \xrightarrow{I} g + X$  cross section, normalized by the total cross section  $\sigma_{q'g}^{(I)}$ . The mean gluon multiplicity [5,10] is then found by phase space integration,

$$\langle n_g \rangle^{(I)} \left( x', \frac{Q'}{\Lambda_{\overline{\text{MS}}}^{(n_f)}}, \frac{\mu_r}{Q'}, n_f \right) = \frac{2\pi}{\alpha_{\overline{\text{MS}}}(1/\rho^*)} (\xi_* - 2) \frac{dS^{(I\bar{I})}}{d\xi}(\xi_*). \quad (13)$$

The function **GMULT** calculates and returns the average gluon multiplicity (13).

The stars (\*) in Eq. (13) denote the saddle point values of the  $I\bar{I}$  collective coordinates  $\rho$ ,  $\bar{\rho}$  and  $\xi$ . Their computation proceeds as in the descriptions of the functions **Q2SIG** and **XI**. The required values of  $4\pi/\alpha_{\overline{\text{MS}}}$  are calculated and returned by the function **XQS**. The  $I\bar{I}$ -action  $S^{(I\bar{I})}(\xi)$  and its  $\xi$ -derivatives are provided by the subroutine **ACTION**.

## SUBROUTINE **HERLUND**

*Purpose:* Conversion of the HERWIG [8] event record in the HEPEVT common block to the respective JETSET [18] common block.

*Remarks:* **HERLUND** is a modified [17] copy from the JETSET subroutine LUHEPC.

## SUBROUTINE **HVHBVI**

*Purpose:* Call of the main (hard) instanton process generator **QIHGEN**.

*Remarks:* Replaces a dummy stub in HERWIG [8] that was originally used as event generation interface for the Monte Carlo generator HERBVI [23] for baryon number violating interactions. Used in the QCDINS package to select QCD-instanton induced processes via  $\text{MOD}(\text{IPROC}/100,100) > 75$ . The process code IPROC (= 17600) has to be set in the user's steering program (c.f. Appendix A). Furthermore, the QCDINS program header is printed.

## SUBROUTINE **HWBJCO**

*Purpose:* Modification of HERWIG [8] routine to account for instanton-induced scattering.

*Remarks:* The modifications are [24]: The logical flag (DISPRO) for keeping the lepton momenta fixed in HERWIG 5.9 is modified to include also instanton-induced DIS, IPRO = 76. Furthermore, a bug concerning energy-momentum conservation in the original routine from HERWIG 5.9 has been fixed.

## SUBROUTINE **HWEGAM** (IHEP, ZMI, ZMA, WWA)

*Purpose:* Modification to avoid standard generation of the (virtual) photon at this stage.

*Arguments:* c.f. Ref. [8]

*Remarks:* This is a modified routine from HERWIG 5.9 (c.f. Ref. [8]). Usually, **HWEGAM** generates an incoming photon from the incoming  $e^\pm$ . Within QCDINS, however, the photon is generated at a later stage in the subroutine **QIKGAM**. Thus, the HERWIG routine **HWEGAM** has been modified to immediately return for instanton-induced processes (IPRO=76).

## FUNCTION **LAMBERTW** (X)

*Purpose:* Calculation of the principal branch of the Lambert W-function  $W(x)$  for  $x \geq 0$ .

*Arguments:* X:  $x \geq 0$ ; argument of the Lambert W-function.

*Procedure:*

$W(x)$  is the (real) solution of  $W(x) \exp(W(x)) = x$ , analytic at  $x = 0$ . The following simple, but accurate approximation is used and returned by **LAMBERTW**:

$$W(x) \approx \begin{cases} 0.665 \cdot (1 + 0.0195 \cdot \ln(x+1)) \ln(x+1) + 0.04; & \text{for } 0 \leq x \leq 500; \\ \ln(x-4) - (1 - \frac{1}{\ln(x)}) \cdot \ln(\ln(x)); & \text{for } x > 500. \end{cases} \quad (14)$$

FUNCTION **LAMNF** (NF, LAMBDA5)

*Purpose:* Calculation of  $\Lambda_{\overline{\text{MS}}}^{(n_f < 5)}$  from  $\Lambda_{\overline{\text{MS}}}^{(5)}$  to order  $\alpha_{\overline{\text{MS}}}^3$ .

*Arguments:*

NF: number of (light) flavours,  $n_f$ .

LAMBDA5: input value  $\Lambda_{\overline{\text{MS}}}^{(5)}$ .

*Procedure:* The flavour reduction of  $\Lambda_{\overline{\text{MS}}}^{(5)}$  to the desired number of light flavours is performed by using Eq. (9.7) of Ref. [16].

SUBROUTINE **LUHEPC** (MCONV)

*Purpose:* Conversion of the JETSET [18] event record contents back to the HEPEVT common block.

*Arguments:* MCONV = 1

*Remarks:* The present routine is a modified [21] version of the JETSET routine **LUHEPC**.

FUNCTION **OMEGA** (XI4)

*Purpose:* Calculation of the fermionic overlap, as function of the conformally invariant  $I\bar{I}$ -distance.

*Arguments:* XI4: conformally invariant  $I\bar{I}$ -distance  $\xi$ .

*Procedure:*

The following simple, but accurate approximation for the fermionic overlap [4]  $\omega$  is used and returned by **OMEGA**:

$$\omega(\xi) \approx \frac{4}{(\xi + 1/2)^{3/2}}. \quad (15)$$

FUNCTION **Q2SIG** (XPRIME, QLAM, KAPPA, LOOPFL, NF)

*Purpose:* Calculation of the total cross section

$$Q'^2 \sigma_{q'g}^{(I)} \quad [\text{nb GeV}^2] \quad (16)$$

for the instanton-induced subprocess, depending on  $x'$ ,  $Q'/\Lambda_{\overline{\text{MS}}}^{(n_f)}$ ,  $\mu_r/Q'$ , loop-order and  $n_f$ . Here,  $\mu_r$  and  $n_f$  denote the renormalization scale and the number of light flavours, respectively.

*Arguments:*

XPRIME:  $x'$

QLAM:  $Q'/\Lambda_{\overline{\text{MS}}}^{(n_f)}$

KAPPA:  $\mu_r/Q'$

LOOPFL: = 1: 1-loop renormalization group (RG) invariance [4] along with 1-loop form of  $\alpha_s$ .

= 2: 2-loop RG invariance [4] along with 2-loop form of  $\alpha_{\overline{\text{MS}}}$ .

= 3: (default) 2-loop RG invariance along with 3-loop form of  $\alpha_{\overline{\text{MS}}}$ .

NF:  $n_f$ ; number of light flavours.

*Procedure:*

The function **Q2SIG** calculates and returns the cross section (16) as derived in Ref. [4],

$$\begin{aligned} Q'^2 \sigma_{q'g}^{(I)} &= d_{\overline{\text{MS}}}^2 \frac{\sqrt{12}}{2^{16}} \pi^{15/2} \frac{((\xi_* + 2)v_*^2 + 4\tilde{S}(\tilde{S} - 2v_*))}{(v_* - \tilde{S})^{9/2} \sqrt{(\xi_* + 2)v_* - 4\tilde{S}}} \left( \frac{(\xi_* - 2)}{\xi_*} \frac{\Delta_1 \beta_0}{D(\tilde{S})} \right)^{7/2} \\ &\times \frac{\omega(\xi_*)^{2n_f-1} (\xi_* - 2)^3 v_*^5}{\sqrt{\frac{1}{2}(\tilde{S} - v_* - 2D(\tilde{S}))^2 + \tilde{S}(\tilde{S} - v_*)D \left( \ln \left( \frac{D(\tilde{S})}{\sqrt{\xi_* - 2}} \right) \right)}} \\ &\times \left( \frac{4\pi}{\alpha_{\overline{\text{MS}}}(\mu_r)} \right)^{19/2} \exp \left[ -\frac{4\pi}{\alpha_{\overline{\text{MS}}}(\mu_r)} S^{(I\bar{I})}(\xi_*) - 2 \left( 1 - \ln \left( \frac{v_* \mu_r}{Q'} \right) \right) \tilde{S} \right]. \end{aligned} \quad (17)$$

It is expressed entirely in terms of the saddle point values for the  $I\bar{I}$  collective coordinates,  $\xi_*$  (conformally invariant distance) and  $v_* \equiv Q'\rho_*$  (scaled size). For given  $x'$ ,  $Q'/\Lambda_{\overline{\text{MS}}}^{(n_f)}$  and (scaled) renormalization scale  $\mu_r/Q'$ , these are in turn unique solutions of the saddle point equations [4]

$$\xi_* - 2 = 4 \frac{x'}{1 - x'} \left( 1 - \frac{\tilde{S}(\xi_*)}{v_*} \right)^2, \quad (18)$$



$$v_* = 2 D(\tilde{S}(\xi_*)) W \left( \frac{Q' \exp \left\{ \frac{1}{2} \left[ \frac{4\pi}{\alpha_{\overline{\text{MS}}}(\mu_r)} \frac{1}{\Delta_1 \beta_0} + \frac{\tilde{S}(\xi_*)}{D(\tilde{S}(\xi_*))} \right] \right\}}{\mu_r \frac{2 D(\tilde{S}(\xi_*))}{\mu_r}} \right), \quad (19)$$

with

$$\Delta_1 = \begin{cases} 1 & \text{for LOOPFL} = 1; \\ 1 + \frac{\beta_1}{\beta_0} \frac{\alpha_{\overline{\text{MS}}}(\mu_r)}{4\pi} & \text{for LOOPFL} = 2, 3; \end{cases} \quad (20)$$

and

$$\Delta_2 = \begin{cases} 0 & \text{for LOOPFL} = 1; \\ 12 \beta_0 \frac{\alpha_{\overline{\text{MS}}}(\mu_r)}{4\pi} & \text{for LOOPFL} = 2, 3. \end{cases} \quad (21)$$

The  $I\bar{I}$ -action  $S^{(I\bar{I})}(\xi)$  as well its  $\xi$ -derivatives, entering the cross section (17) and Eqs. (18), (19) through

$$\tilde{S}(\xi_*) \equiv \Delta_1 \beta_0 S^{(I\bar{I})}(\xi_*) - \Delta_2; \quad D(f(\xi_*)) \equiv \frac{d}{d \ln(\xi_* - 2)} f(\xi_*), \quad (22)$$

are calculated in the subroutine **ACTION**. The fermionic overlap  $\omega(\xi)$  is calculated and returned by the function **OMEGA**. In Eq. (19),  $W$  denotes the principal branch of the Lambert  $W$ -function, i.e. the (real) solution of  $W(x) \exp(W(x)) = x$ , analytic at  $x = 0$ . The latter is calculated and returned by the function **LAMBERTW**.

The first step in the solution of the saddle-point equations (18), (19) consists in eliminating  $v_*$  in Eq. (18) by inserting Eq. (19). Next, for given  $x'$ ,  $Q'/\Lambda_{\overline{\text{MS}}}^{(n_f)}$  and  $\mu_r/Q'$ , the resulting implicit equation is solved numerically for  $\xi_*$ . This is done by the function **XI** which provides  $\xi_* = \xi_*(x', Q'/\Lambda_{\overline{\text{MS}}}^{(n_f)}, \mu_r/Q')$  on return. The latter is then inserted into Eq. (19) providing  $v_* = v_*(x', Q'/\Lambda_{\overline{\text{MS}}}^{(n_f)}, \mu_r/Q')$ .

The values of  $4\pi/\alpha_{\overline{\text{MS}}}$  are calculated and returned by the function **XQS**.

#### SUBROUTINE **QCDGEN**

*Purpose:* Interface for the generation of one instanton-induced event, including calls to event initialization, hadronization and event termination routines.

*Procedure:*

- An instanton-induced event is initialized by a call to the HERWIG [8] subroutine **HWUINE**.
- The partonic instanton subprocess is generated by a call to the HERWIG subroutine **HWEPRO**.
- If the hadronization flag QICONT(21) is set .TRUE. (default), the event is fully hadronized. Else, the event is finalized (**HWUFNE**) immediately after the call of **HWEPRO**. Depending on the control flag for the hadronization model, QICONT(18)=.TRUE./.FALSE., the hadronization is either performed by appropriate HERWIG [8] or (modified [17]) JETSET [18] routines, respectively (see Table 3).
- Furthermore, in this routine energy-momentum conservation in the generated event is checked.

### SUBROUTINE QCLOOP

*Purpose:* Loop over calls to the instanton event generator and interface of the instanton-induced hard subprocess to HERWIG [8] initialization and output routines.

*Procedure:*

- The instanton-induced hard subprocess is initialized by calling the HERWIG subroutine **HWEINI**.
- The generator **QCDGEN** for an instanton-induced event and, thereafter, the user's routine **HWANAL** for analyzing data from the event, are called in a loop MAXEV times, with MAXEV being the desired number of events. MAXEV has to be set in the user's steering program (c.f. Appendix A).
- The instanton-induced hard subprocess is terminated by calling the HERWIG subroutine **HWEFIN** that produces the final output.

### SUBROUTINE QICALC

*Purpose:* Calculates derived parameters and checks the chosen kinematical boundaries. The latter are adjusted in case of inconsistencies.

*Non-local variables (re)set:*

QILPAR(I):	= LOG(QIUPAR(I)), I = 1 .. 18, if QIUPAR(I) > 1.0 · 10 <sup>-20</sup> ; otherwise QILPAR(I) = -1.0 · 10 <sup>25</sup> ; these parameter settings are partially re-set after exit (see below).
QIDPAR(1):	= QIUPAR(12)**2; square of minimum allowed instanton CM energy $W_{I\min}^2$ .
QIWARF(1):	= .FALSE. (default); if $Q_{\max}'^2$ violates the kinematical constraint

$$Q_{\max}'^2 \leq z_{\max} S - W_{I\min}^2, \quad (23)$$

QICONT(18)	Hadronization scheme	
.TRUE.	HERWIG Interface	
	<b>HWUINE</b>	Initialize event
	<b>HWEPRO</b>	Generate hard subprocess
	<b>HWBGEN</b>	Generate parton cascades
	<b>HWDHQQ</b>	Do heavy quark decays
	<b>HWCFOR</b>	Do cluster hadronization
	<b>HCWDEC</b>	Do cluster decay
	<b>HWDHAD</b>	Do unstable particle decays
	<b>HWDHVV</b>	Do heavy flavour decays
	<b>HWMEVT</b>	Add soft underlying event if needed
	<b>HWUFNE</b>	Finalize event
.FALSE.	JETSET Interface	
	<b>HWUINE</b>	Initialize event
	<b>HWEPRO</b>	Generate hard subprocess
	<b>HWBGEN</b>	Generate parton cascades
	<b>HWUFNE</b>	Finalize event
	<b>HERLUND</b>	Convert HERWIG event record in HEPEVT common block to the respective JETSET common block
	<b>LUGIVE</b>	Assign the hard subprocess (HARD) and instanton (INST) character strings in JETSET common block
	<b>LUEXEC</b>	Simulate the whole fragmentation and decay chain
	<b>LULIST(1)</b>	List the (first) event record
	<b>LUHEPC(1)</b>	Convert JETSET event record contents back to the HEPEVT common block

Table 3

Depending on the flag  $\text{QICONT}(18) = \text{.TRUE./FALSE.}$ , HERWIG [8] and JETSET [18] hadronization may be selected. The respective calls to HERWIG and (modified) JETSET routines used in **QCDGEN** are displayed.

	QIWARF(1) is reset to .TRUE..
QINWAR(1):	= 0 (default); counts the number of violations of Eq. (23).
QILPAR(8):	= $\ln Q_{\max}^{\prime 2}$ (default); reset to the logarithm of the right hand side of Eq. (23) if this kinematical constraint is violated.
QIUPAR(8):	= $Q_{\max}^{\prime 2}$ ; reset to the right hand side of Eq. (23) if this kinematical constraint is violated.
QIWARF(2):	= .FALSE. (default); if $Q_{\min}^{\prime 2}$ violates the kinematical constraint

$$Q_{\min}^{\prime 2} \geq \frac{x_{\text{Bj min}}}{z_{\max} - x_{\text{Bj min}}} W_{I \min}^2, \quad (24)$$

	QIWARF(2) is reset to .TRUE..
QINWAR(2):	= 0 (default); counts the number of violations of Eq. (24).
QILPAR(9):	= $\ln Q_{\min}^{\prime 2}$ (default); reset to the logarithm of the right hand side of Eq. (24) if this kinematical constraint is violated.
QIUPAR(9):	= $Q_{\min}^{\prime 2}$ ; reset to the right hand side of Eq. (24) if this kinematical constraint is violated.
QIWARF(3):	= .FALSE. (default); if $x'_{\max}$ violates the kinematical constraint

$$x'_{\max} \leq 1 - \frac{W_{I \min}^2}{z_{\max} S}, \quad (25)$$

	QIWARF(3) is reset to .TRUE..
QINWAR(3):	= 0 (default); counts the number of violations of Eq. (25).
QILPAR(6):	= $\ln x'_{\max}$ (default); reset to the logarithm of the right hand side of Eq. (25) if this kinematical constraint is violated.
QIUPAR(6):	= $x'_{\max}$ ; reset to the right hand side of Eq. (25) if this kinematical constraint is violated.
QIWARF(4):	= .FALSE. (default); if $x'_{\min}$ violates the kinematical constraint

$$x'_{\min} \geq \frac{x_{\text{Bj min}}}{z_{\max}}, \quad (26)$$

	QIWARF(4) is reset to .TRUE..
QINWAR(4):	= 0 (default); counts the number of violations of Eq. (26).
QILPAR(7):	= $\ln x'_{\min}$ (default); reset to the logarithm of the right hand side of Eq. (26) if this kinematical constraint is violated.

QIUPAR(7):	$= x'_{\min}$ ; reset to the right hand side of Eq. (26) if this kinematical constraint is violated.
QIWARF(11):	$= .FALSE.$ (default); reset to $.TRUE.$ if current quark mass requirement (c. f. QICON(6)) does not fit to the selected order of variable generation (c. f. QICON(5)).
QINWAR(11):	$= 0$ (default); counts the number of recurring QIWARF(11) $= .TRUE.$ settings.
QICON(6):	$= .TRUE.$ (default); reset to $.FALSE.$ if the flag QIWARF(11) $= .TRUE.$ .
QIQMASS(1,I):	$\sum_{i=1}^I m_{q_i}$ ; cumulative sum of HERWIG [8] quark masses with $1 \leq I \leq 6$ referring to the HERWIG identity code.
QIQMASS(2,I):	$m_{q_i}$ ; HERWIG quark mass with $1 \leq I \leq 6$ referring to the HERWIG identity code.
QIRCAL:	$= .TRUE.$ (default); reset to $.FALSE.$ on exit.

*Remarks:* This routine is only performed if the flag QIRCAL is set to  $.TRUE.$  (**QIINIT**, **QISETD**, **QISETF**, **QISETI**).

#### SUBROUTINE QICCON

*Purpose:* Assignment of the colour and flavour connections for the partons.

*Non-local variables (re)set:*

QIPLIS (JLP, ILP):	IHEP pointer referring to the outgoing parton JLP in the string ILP.
JMOHEP:	array of HERWIG [8] “mother” pointers.
JDAHEP:	array of HERWIG “daughter” pointers.

*Remarks:* For an explicit example, see the description of routine **QISTID**.  
*Procedure:*

- The IHEP pointer of the current quark  $k$  (IHEP=10), as assigned in **QIHGEN**, is added to the array QIPLIS of IHEP pointers at the position (JLP,ILP) of the virtual quark  $q'$ .
- The IHEP pointer of the incoming gluon (IHEP=6), as assigned in **QIHGEN**, is added to the array QIPLIS of IHEP pointers at the position (JLP,ILP) of the incoming gluon.
- The colour flow is constructed by connecting the colour lines of neighbouring partons within each of the strings constructed in the subroutines **QIGLST** and **QIGPAR**.
- Finally, the flavour flow is constructed by connecting the flavour lines of the quark at the beginning of a string with the flavour line of the anti-quark at the end of a string.

SUBROUTINE **QIGETD** (NUM, VALUE, OK)

*Purpose:* Get value of double precision parameter QIUPAR(NUM) for given NUM.

*Arguments:*

NUM: integer, pointing to the parameter QIUPAR(NUM) to be read.

VALUE: value of double precision parameter QIUPAR(NUM).

OK: logical return flag.

*Non-local variables (re)set:*

QINWAR(10): = QINWAR(10)+1; counts attempts to read non-existing parameter QIUPAR(.).

QIWARF(10): = .TRUE. if parameter index NUM out of range.

*Remarks:* Service routine for reading out the double precision input parameters QIUPAR(NUM), NUM=1,2,...,18. On return, the logical flag OK is .TRUE. if NUM is within its allowed range.

SUBROUTINE **QIGETF** (NUM, FLAG, OK)

*Purpose:* Get value of logical flag QICONT(NUM) for given NUM.

*Arguments:*

NUM: integer, pointing to the parameter QICONT(NUM) to be read.

FLAG: boolean value of QICONT(NUM).

OK: logical return flag.

*Non-local variables (re)set:*

QINWAR(6): = QINWAR(6)+1; counts attempts to read non-existing parameter QICONT(.).

QIWARF(6): = .TRUE. if parameter index NUM out of range.

QIRCAL: = .TRUE. if QIWARF(6) = .FALSE. (default).

*Remarks:* Service routine for reading out the boolean input parameters QICONT(NUM), NUM=1,2,...,21. On return, the logical flag OK is .TRUE. if NUM is within its allowed range.

SUBROUTINE **QIGETI** (NUM, VALUE, OK)

*Purpose:* Get value of integer parameter QIPARI(NUM) for given NUM.

*Arguments:*

NUM: integer, pointing to the parameter QIPARI(NUM) to be read.

VALUE: value of QIPARI(NUM).

OK: logical return flag.

*Non-local variables (re)set:*

QINWAR(8): = QINWAR(8)+1; counts attempts to read non-existing parameter QIPARI(.).  
 QIWARF(8): = .TRUE. if parameter index NUM out of range.  
 QIRCAL: = .TRUE. if QIWARF(8) = .FALSE. (default).

*Remarks:* Service routine for reading out the integer input parameters QIPARI(NUM), NUM=1,2,...,10. On return, the logical flag OK is .TRUE. if NUM is within its allowed range.

## SUBROUTINE QIGLST

*Purpose:* Generation of  $n_f [q \dots \bar{q}]$  - “strings” of partons, with a total number  $n_g+1$  of gluons inserted in between, in accord with the requirement of “flavour democracy” among the  $n_f q\bar{q}$ -pairs participating in the instanton-induced subprocess.

*Non-local variables (re)set:*

QIPTYP (JLP, ILP): particle data group [16] identity code (IDPDG) of the parton JLP in the string ILP.  
 QINLIS (ILP): number of partons in the string ILP.  
 QIPINF (JLP, ILP): = .FALSE.; logical flag indicating whether parton JLP in the string ILP is incoming.

*Procedure:*

Each of the  $n_f$  generated strings begins with a quark, followed by a random number  $\leq n_g + 1$  of gluons, and ends with an anti-quark of randomly chosen flavour. Due to the required “flavour democracy”,  $q\bar{q}$ -pairs of all  $n_f$  flavours must occur precisely once, e. g. for  $n_f = 3$  and  $n_g = 3$ ,

$$[d \, g \, \bar{u}] \quad [u \, g \, g \, \bar{s}] \quad [s \, g \, \bar{d}]. \quad (27)$$

In practice, the strings are generated and administrated as follows:

- First, a 2-dimensional integer array QIPTYP is defined, whose entries QIPTYP (JLP, ILP) will contain the particle data group identity code (IDPDG) of the parton JLP in the ILP-th  $[q \dots \bar{q}]$  - string. All entries are initially set to zero.
- The quarks, labelled by their IDPDG-codes  $1..n_f$ , are then inserted con-

secutively at the top of the first  $n_f$  columns (“strings”), e. g. for  $n_f = 3$ ,

		ILP					
		1	2	3	4	.	30
JLP	1	1	2	3	0	.	0
	2	0	0	0	0	.	0
	.	.	.	.	.	.	.
	30	0	0	0	0	.	0
	QINLIS(ILP)	1	1	1	0	.	0

- Next, the anti-quarks with IDPDG-codes  $-1 \dots -n_f$ , are inserted randomly in the second row of the first  $n_f$  columns, e.g.

		ILP					
		1	2	3	4	.	30
JLP	1	1	2	3	0	.	0
	2	-2	-3	-1	0	.	0
	3	0	0	0	0	.	.
	.	.	.	.	.	.	.
	30	0	0	0	0	.	0
	QINLIS(ILP)	2	2	2	0	.	0

- Finally, the  $n_g + 1$  gluons of the instanton subprocess with IDPDG-code 21 are distributed randomly over the first  $n_f$  columns in between the quarks and anti-quarks: For each of the gluons, one of the first  $n_f$  columns is picked at random, the anti-quark in this column is moved one row further down and the gluon is inserted at the anti-quark’s previous position. A possible outcome of this procedure for the example above with  $n_g = 3$  is

		ILP					
		1	2	3	4	.	30
JLP	1	1	2	3	0	.	0
	2	21	21	21	0	.	0
	3	-2	21	-1	0	.	.
	4	0	-3	0	0	.	.
	5	0	0	0	0	.	.
	.	.	.	.	.	.	.
	30	0	0	0	0	.	0
	QINLIS(ILP)	3	4	3	0	.	0

SUBROUTINE **QIGMUL** (WGTFCT)



*Purpose:* Generation of the number of gluons  $n_g$  emitted by the instanton subprocess in accord with kinematical constraints.

*Arguments:*

WGTFCT: = 1.0, returned, if the event is to be accepted.  
= 0.0, returned, if the final state quark masses are too high; event will be killed (default).

*Non-local variables (re)set:*

QINGLU:  $n_g + 1$ , number of gluons involved in the instanton subprocess.  
QIWARF(14): = .FALSE. (default); reset to .TRUE. if the calculation of the number of gluons requires too many iterations.  
QINWAR(14): = 0 (default); counts the number of recurring QIWARF(14) = .TRUE. settings.

*Procedure:*

- The minimal CM energy available for gluon generation is calculated and WGTFCT is set accordingly.
- If the emission of at least one gluon is energetically allowed, the average gluon multiplicity  $\langle n_g \rangle^{(I)}$  is calculated and returned by the function **GMULT**.
- The number  $n_g$  of emitted gluons is then generated according to a Poisson distribution [9] with mean  $\langle n_g \rangle^{(I)}$ ,

$$P(n_g) = \frac{\langle n_g \rangle^{(I) n_g}}{n_g!} e^{-\langle n_g \rangle^{(I)}}. \quad (28)$$

- An upper limit on  $\langle n_g \rangle^{(I)}$  is enforced and the kinematical constraints are checked again. In case they are violated, a new iteration cycle is started corresponding to a different generated value of  $n_g$ .

## SUBROUTINE QIGPAR

*Purpose:* Identification of the incoming partons among the partons participating in the instanton-induced subprocess.

*Non-local variables (re)set:*

QIPINC(1,1): row number (JLP) in the 2-dimensional array QIPTYP (**QIGLST**), where the anti-parton corresponding to the incoming virtual (anti-)quark  $q'$  is located.

QIPINC(1,2):	column number (ILP) in the 2-dimensional array QIPTYP ( <b>QIGLST</b> ), where the anti-parton corresponding to the incoming virtual (anti-)quark $q'$ is located.
QIPINC(2,1):	row number (JLP) of the incoming on-shell gluon $g$ in the 2-dimensional array QIPTYP ( <b>QIGLST</b> ).
QIPINC(2,2):	column number (ILP) of the incoming on-shell gluon $g$ in the 2-dimensional array QIPTYP ( <b>QIGLST</b> ).
QIPINF(JLP, ILP):	= .FALSE. (default); set to .TRUE. only if (JLP, ILP) = (QIPINC(I,1), QIPINC(I,2)), with I=1,2, corresponding to the incoming partons.

*Procedure:*

One of the  $n_g + 1$  gluons in the generated  $n_f [q \dots \bar{q}]$ -strings (**QIGPAR**) is randomly chosen and marked as incoming. Furthermore, the anti-parton corresponding to the virtual (anti-)quark  $q'$  is identified and marked as incoming.

## SUBROUTINE **QIHGEN**

*Purpose:* Main (hard) instanton process generator.

*Non-local variables (re)set:*

QISGAM:	$eP$ CM energy squared $S$ .
IDN(1):	HERWIG identity code (IDHW) of incoming $e$ .
IDN(2):	HERWIG identity code (IDHW) of incoming $g$ .
EMSCA:	factorization scale $\mu_f = \text{QIUPAR}(18)$
QIZPAR:	generated $z$ .
QIXONE:	$x' z$
QIYONE:	$Q'^2 / (S x' z)$
QIXBJG:	generated $x_{\text{Bj}}$ .
QIYBJG:	generated $y_{\text{Bj}}$ .
QIQ2GA:	Bjorken variable $Q^2$ calculated via $Q^2 = S x_{\text{Bj}} y_{\text{Bj}}$ .
QIELEN:	energy of incoming $e$ , $e_t$ .
QIPREN:	energy of incoming $P$ , $P_t$ .
EVWGT:	weight $W_{eP}^{(I)}$ (39) corresponding to the instanton-induced cross section (3).
QIMEWT:	internal storage of weight corresponding to Eq. (3) for analysis
QIPINC(1,3):	particle data group identity code (IDPDG) of virtual quark $q'$ .

QIPINC(2,3):	particle data group identity code (IDPDG) of incoming gluon $g$ .
QIPINC(1,4):	(=10) IHEP pointer of current quark $k$ .
QIPINC(2,4):	(=6) IHEP pointer of incoming $g$ .
QISHEP:	CM energy squared of instanton subprocess, $W_I^2 = (q' + g)^2 = s'$ .
JMOHEP:	array of HERWIG [8] “mother” pointers.
JDAHEP:	array of HERWIG “daughter” pointers.

*Procedure:*

For the generation of an event, this routine is called twice: in the first call, a Monte Carlo weight associated with the instanton-induced total cross section is calculated. In the second call, the generation of the event is completed.

In the first call (GENEV = .FALSE.), the following steps are performed in **QIHGEN**:

- Information on the incoming beams is accumulated, initial state radiation from the lepton is optionally accounted for (**EXFRAC**), various derived parameters are calculated and kinematical limits are checked (**QICALC**).
- The HERWIG [8] identity code (IDHW) of the current quark  $k$  and of the virtual quark  $q'$  (c.f. Fig. 1) are generated (**QIHPAR**).
- Next follows the generation of the various Bjorken variables  $Q'^2$ ,  $x'$ ,  $z$ ,  $x_{\text{Bj}}$ ,  $y_{\text{Bj}}$  (c.f. Fig. 1) of the instanton-induced DIS process, with weights corresponding to the associated factors appearing in the instanton-induced total cross section (3):
  - By a call to **QIHINS**, the Bjorken variables  $Q'^2$  and  $x'$  of the instanton subprocess are generated. Moreover, the Monte Carlo weight  $W_{Q'x'\sigma}$  from Eq. (43), corresponding to the integral

$$\int_{Q'^2_{\min}}^{Q'^2_{\max}} dQ'^2 \int_{x'_{\min}}^{x'_{\max}} \frac{dx'}{x'} \frac{2}{x'} \sigma_{q'g}^{(I)}(x', Q'^2), \quad (29)$$

is calculated, where  $\sigma_{q'g}^{(I)}$  denotes the instanton-induced  $q'g$  total cross section [4] from Eq. (17). At this stage, also the gluon multiplicity depending on  $x'$  and  $Q'^2$  is generated (**QIGMUL**).

- The fractional momentum  $z$  of the incoming gluon is generated and the Monte Carlo weight  $W_{zg}$  corresponding to the integral

$$\int_{\max\left(\frac{Q'^2}{Sx'y_{\text{Bj max}}}, \frac{x_{\text{Bj min}}}{x'}\right)}^{z_{\max}} dz f_g(z, \mu_f), \quad (30)$$

is calculated, where  $f_g$  is the gluon distribution in the proton. By default,  $f_g$  is taken from Ref. [25] (set 1.1) and the factorization scale  $\mu_f$  is identified with  $Q'_{\min}$ . For the default setting of the control flags in **QUINIT**, the value of  $z$  as well as the Monte Carlo weight  $W_{zg}$  are generated as follows: Random points  $y_z$ , with

$$y_z = \ln z \quad \Leftrightarrow \quad z = \exp y_z \quad (31)$$

are generated uniformly in the interval between  $\ln z_L$  and  $\ln z_U$ , where  $z_L$  and  $z_U$  are the lower and upper integration limits in Eq. (30), respectively. Hence, the Monte Carlo weight associated with Eq. (30) reads

$$W_{zg} = (\ln z_U - \ln z_L) z f_g(z, \mu_f). \quad (32)$$

- The Bjorken variables  $x_{\text{Bj}}$  and  $y_{\text{Bj}}$  are generated analogously to the  $z$  variable and the weight  $W_{x_{\text{Bj}} y_{\text{Bj}}}$ ,

$$W_{x_{\text{Bj}} y_{\text{Bj}}} = \ln \frac{x_{\text{Bj} U}}{x_{\text{Bj} L}} \ln \frac{y_{\text{Bj} U}}{y_{\text{Bj} L}} \theta(S x_{\text{Bj}} y_{\text{Bj}} - Q_{\min}^2), \quad (33)$$

corresponding to the integral

$$\int_{x_{\text{Bj} L}}^{x_{\text{Bj} U}} \frac{dx_{\text{Bj}}}{x_{\text{Bj}}} \int_{y_{\text{Bj} L}}^{y_{\text{Bj} U}} \frac{dy_{\text{Bj}}}{y_{\text{Bj}}} \theta(S x_{\text{Bj}} y_{\text{Bj}} - Q_{\min}^2) \quad (34)$$

is calculated. The integration limits in Eq. (34) are given in terms of the physical  $x_{\text{Bj}}$ ,  $y_{\text{Bj}}$ -cuts, with default values as displayed in Table 4,

$$\begin{aligned} x_{\text{Bj} U} &= x' z - \frac{m_k^2}{S} \frac{1}{y_{\text{Bj} \max} - \frac{Q'^2}{S x' z}}; \\ x_{\text{Bj} L} &= x_{\text{Bj} \min}; \\ y_{\text{Bj} U} &= y_{\text{Bj} \max}; \\ y_{\text{Bj} L} &= \max \left( \frac{Q'^2}{S x' z} + \frac{m_k^2}{S} \frac{1}{x' z - x_{\text{Bj}}}, y_{\text{Bj} \min} \right). \end{aligned} \quad (35)$$

- Finally, given the generated Bjorken variables, the weights associated with the remaining factors in the instanton-induced cross section (3) are calculated:

- The weight arising from the splitting of the photon into a  $q\bar{q}$ -pair is obtained from the routine **QISPLT**,

$$W_{q'} = \frac{1}{x' z} P_{q'}^{(I)}(x', Q'^2, z, Q^2 = S x_{\text{Bj}} y_{\text{Bj}}). \quad (36)$$

The factor  $P_{q'}^{(I)}$  from Eq. (4) accounts for the flux of virtual (anti-)quarks  $q'$  in the instanton background, entering the instanton-induced  $q'g$ -subprocess from the photon side [4,14] (c.f. Fig. 1).

- The familiar weight from the flux of virtual photons is calculated,

$$W_\gamma = \frac{1}{S x_{\text{Bj}} y_{\text{Bj}}} \left( 1 - y_{\text{Bj}} + \frac{y_{\text{Bj}}^2}{2} \right). \quad (37)$$

- The left-over weight factor required for a properly normalized cross section (in units of nb) is obtained from the routine **QIPVWT**,

$$W_n = 2 \pi \alpha^2 x_{\text{Bj}} x' \sum_{q'=d,u,s,\dots; \bar{d},\bar{u},\bar{s},\dots} e_{q'}^2. \quad (38)$$

Here  $\alpha$  is the electro-magnetic fine-structure constant and  $e_{q'}$  denotes the fractional electro-magnetic charge of the virtual (anti-)quark  $q'$ . The sum extends over quarks and anti-quarks of the considered  $n_f$  light flavours.

- The total event weight (EVWGT) required by the HERWIG package, is the product of all the above weights,

$$W_{eP}^{(I)} = W_{Q'x'\sigma} W_{zg} W_{x_{\text{Bj}} y_{\text{Bj}}} W_{q'} W_\gamma W_n. \quad (39)$$

This ends the first call of **QIHGEN**.

For standard settings of the control flags in the HERWIG [8] routine **HWIGIN** (NOWGT=.TRUE.), the (standard) rejection method is applied producing an unweighted event distribution according to the instanton-induced, normalized differential cross section (9).

If the event is accepted (GENEV = .TRUE.), **QIHGEN** is called again. The following steps are then performed:

- The lepton beam  $e$  is stored in the event record.
- The 4-momentum  $g$  of the incoming gluon is calculated from its generated fractional momentum  $z$  and the 4-momentum of the incoming proton (**QIKPAR**). The result is stored in the event record.
- The 4-momentum  $q$  of the virtual photon is generated (**QIKGAM**).
- The 4-momentum  $e'$  of the outgoing lepton is calculated from  $e, q$  and stored.
- The 4-momenta of the virtual quark  $q'$  and the outgoing current quark  $k$  are generated (**QIKGSP**) and copied into the event record.
- The required data for the generation routines of the instanton subprocess

$$q'g \xrightarrow{I} X \quad (40)$$

are set up and its (total) momentum vector  $q' + g$  is calculated.

- The colour connections of the hard subprocess are initiated.
- The instanton-induced partonic final state  $X$  in Eq. (40) is generated (**QISTID**) with all colour connections in the  $q'g$ -CM system and, thereafter, transformed into the laboratory frame.

## SUBROUTINE **QIHINS**

*Purpose:* Generation of the Bjorken variables  $Q'^2$  and  $x'$ , associated with the instanton subprocess, and calculation of the Monte Carlo weight associated with the integral (29).

*Non-local variables (re)set:*

**QIL2IN:**  $Q'^2$  according to Eq. (41).

**QIX1HT:**  $x'$  according to Eq. (41).

**QIWGT:** weight (43) associated with the integral (29).

*Procedure:*

The theoretical distributions in  $Q'^2$  and  $x'$  are very strongly varying functions. Therefore, the improved generation strategy outlined in the description of the routine **QIRDIS** is used for default settings of the control flags in **QIINIT**.

The variables  $Q'^2$  and  $x'$  are generated by calls to the subroutine **QIRDIS**, which provides values of

$$Q'^2 = (Z_{Q'^2})^{-1/N_{Q'^2}} \text{ and } x' = (Z_{x'})^{-1/N_{x'}}, \quad (41)$$

with  $Z_{Q'^2}$  and  $Z_{x'}$  uniformly distributed in the intervals

$$\frac{1}{(Q'^2_{\max})^{N_{Q'^2}}} \leq Z_{Q'^2} \leq \frac{1}{(Q'^2_{\min})^{N_{Q'^2}}} \text{ and } \frac{1}{(x'_{\max})^{N_{x'}}} \leq Z_{x'} \leq \frac{1}{(x'_{\min})^{N_{x'}}}, \quad (42)$$

respectively. The optimal powers  $N_{Q'^2}$  (L2NV) and  $N_{x'}$  (XPNV) are empirically determined and set in **QIHINS**.

In analogy to Eq. (67), the total weight  $W_{Q'x'\sigma}$ , associated with the integral (29), is given as a product of three weight factors

$$W_{Q'x'\sigma} = W_{Q'^2} W_{x'} W_{\sigma}, \quad (43)$$

where

$$W_{Q'^2} = \frac{1}{N_{Q'^2}} \left[ (Q'^2_{\min})^{-N_{Q'^2}} - (Q'^2_{\max})^{-N_{Q'^2}} \right] \frac{1}{(Q'^2)^{-N_{Q'^2}}}; \quad (44)$$

$$W_{x'} = \frac{1}{N_{x'}} \left[ (x'_{\min})^{-N_{x'}} - (x'_{\max})^{-N_{x'}} \right] \frac{1}{(x')^{-N_{x'}}}; \quad (45)$$

$$W_{\sigma} = \frac{2}{x'} Q'^2 \sigma_{q'g}^{(I)}(x', Q'^2). \quad (46)$$

The function **Q2SIG** is invoked to calculate the weight factor (46) from the instanton-induced  $q'g$  total cross section.

## SUBROUTINE **QIHPAR**

*Purpose:* Generation of the HERWIG [8] identity codes (IDHW) of the current quark  $k$  as well as of the virtual quark  $q'$ .

*Non-local variables (re)set:*

QINFAM: = QIPARI(4); number of (light) flavours  $n_f$ .  
QIPINT(1): IDHW of current quark  $k$ .  
QIPINT(2): IDHW of virtual quark  $q'$ .  
QICQM2:  $m_k^2$ ; HERWIG mass squared of current quark.

*Procedure:*

By means of the rejection method, the identity code IDHW of the current quark or anti-quark  $k$  is chosen randomly among  $2n_f$  light quarks and anti-quarks,  $\{d, u, s, \dots; \bar{d}, \bar{u}, \bar{s}, \dots\}$ , according to the probability distribution

$$\frac{e_i^2}{\sum_{q=d,u,\dots;\bar{d},\bar{u},\dots} e_q^2}; \quad i = d, u, \dots; \bar{d}, \bar{u}, \dots, \quad (47)$$

reflecting the flavour structure of the standard electromagnetic  $\gamma q_i \bar{q}_i$ -coupling. The identity code of the virtual quark  $q'$  is then given in terms of IDHW( $k$ ). In Eq. (47),  $e_i$  is the electric charge of the quark flavour  $i$ .

## SUBROUTINE **QIINI**

*Purpose:* Initialization of “particle” ‘INST’ in HERWIG [8] event record.

*Procedure:* Association of the name ‘INST’ with the HERWIG identity code (IDHW) ‘206’ of the instanton “particle” in the HERWIG event record.

## SUBROUTINE **QIINIT**

*Purpose:* Initialization of input parameters as displayed in Tables 4 and 5.

*Procedure:*

The routine is designed to make the changing of default values as easy as possible. The parameters available to the user are listed in Tables 4 and 5 (for the definition of kinematic variables see Fig. 1). Furthermore, a name for the “instanton particle” is set by QIPARC(1)=‘INST’. After setting the parameters, **QIINIT** calls the subroutine **QIINI** to initialize the new instanton particle in the HERWIG event record. Finally, it sets the flag QIRCAL = .TRUE. ( $\Leftrightarrow$  calculate derived quantities and check limits).

Name	Default value	Description
QIUPAR(1)	0.75	Effective gluon mass
QIUPAR(2)	$1.0 \cdot 10^{-3}$	$x_{\text{Bj min}}$ : minimum allowed $x_{\text{Bj}}$
QIUPAR(3)	1.0	$z_{\text{max}}$ : maximum of momentum fraction $z$ carried by the gluon
QIUPAR(4)	1.0	$y_{\text{Bj max}}$ : maximum allowed $y_{\text{Bj}}$
QIUPAR(5)	0.1	$y_{\text{Bj min}}$ : minimum allowed $y_{\text{Bj}}$
QIUPAR(6)	0.9	$x'_{\text{max}}$ : maximum allowed $x'$
QIUPAR(7)	0.35	$x'_{\text{min}}$ : minimum allowed $x'$
QIUPAR(8)	$(\sqrt{\text{QIUPAR}(9)} + 30)^2$	$Q'^2_{\text{max}}$ : maximum allowed $Q'^2$
QIUPAR(9)	$\left(8 \frac{\text{QIUPAR}(13)}{\text{LAMNF}(3,0.15267)}\right)^2$	$Q'^2_{\text{min}}$ : minimum allowed $Q'^2$
QIUPAR(10)	QIUPAR(7)	Cut on $x'$ below which the cross section is assumed constant
QIUPAR(11)	$-1.0 \cdot 10^{-10}$	Minimum allowed weight for exit of main weight generation
QIUPAR(12)	0.0	$W_{I \text{ min}}$ : minimum allowed instanton CM energy
QIUPAR(13)	LAMNF(QIPARI(4),0.219)	$\Lambda_{\overline{\text{MS}}}^{(n_f)}$ : from input value (3 loop) $\Lambda_{\overline{\text{MS}}}^{(5)} = 0.219^{+0.025}_{-0.023}$ GeV [16]
QIUPAR(15)	0.0	Minimum energy after mass subtraction from instanton
QIUPAR(16)	0.15	$\mu_r/Q'$ : renorm. scale in $Q'$ units
QIUPAR(17)	QIUPAR(9)	$Q'^2_{\text{min}}$ : minimum allowed $Q'^2$
QIUPAR(18)	$\sqrt{\text{QIUPAR}(9)}$	$\mu_f$ : factorization scale
QIPARI(1)	206	HERWIG [8] identity code (IDHW) of instanton “particle”
QIPARI(2)	100	Maximum number of MAMBO iterations per weight
QIPARI(3)	300	Maximum number of phase space iterations per MAMBO weight
QIPARI(4)	3	$n_f$ : number of (light) flavours
QIPARI(6)	10	Maximum allowed average gluon multiplicity
QIPARI(7)	20	Maximum number of iterations in the cross section weight generation step
QIPARI(9)	40	Maximum number of <b>QIGMUL</b> iterations
QIPARI(10)	3	Number of loops in $\alpha_{\overline{\text{MS}}}$ evaluation
QINWAR(I)	0	Counts recurrence of warning I, I = 1 .. 14 (c. f. Table 5)

Table 4

Floating point and integer parameters set in **QIINIT**. All energy/mass dimensions are in GeV



Name	Default	Description
QICONT(1)	T	Use non-trivial kinematic weight for given phase space distribution
QICONT(2)	T	Use standard routine (leading-order) to generate weight for given phase space distribution
QICONT(3)	T	Use weight due to instanton cross section
QICONT(4)	T	Disregard instanton minimum mass requirement
QICONT(5)	T	Generate $Q'^2$ before $x'$
QICONT(6)	T	Enforce mass of current quark in kinematics
QICONT(9)	T	Enforce maximum allowed number of gluons
QICONT(11)	T	Check that energy suffices for gluon generation
QICONT(13)	T	Kill events with mass too high
QICONT(14)	T	Use $z$ generation as $dz/z$
QICONT(15)	T	Generate $x'$ with efficiency parametrization
QICONT(16)	T	Generate $Q'^2$ with efficiency parametrization
QICONT(18)	T	Use HERWIG rather than JETSET hadronization
QICONT(20)	T	Azimuthal angle of $e'$ generated randomly
QICONT(21)	T	Full hadronization on/off
QIWARF(1)	F	$Q'^2$ upper generation limit reset
QIWARF(2)	F	$Q'^2$ lower generation limit reset
QIWARF(3)	F	$x'$ upper generation limit reset
QIWARF(4)	F	$x'$ lower generation limit reset
QIWARF(5)	F	Attempt to (re)set non-existent logical parameter ( <b>QISETF</b> )
QIWARF(6)	F	Attempt to read non-existent logical parameter ( <b>QIGETF</b> )
QIWARF(7)	F	Attempt to (re)set non-existent integer parameter ( <b>QISETI</b> )
QIWARF(8)	F	Attempt to read non-existent integer parameter ( <b>QIGETI</b> )
QIWARF(9)	F	Attempt to (re)set non-existent double precision parameter ( <b>QISETD</b> )
QIWARF(10)	F	Attempt to read non-existent double precision parameter ( <b>QIGETD</b> )
QIWARF(11)	F	Current quark mass requirement does not fit to the selected order of variable generation (c.f. QICONT(5))
QIWARF(12)	F	Negative $k_T^2$ for current quark, reset to 0.0
QIWARF(14)	F	Too many iterations in <b>QIGMUL</b>
QIRCAL	T	Check kinematical limits

Table 5

Logical flags set in **QIINIT** (T = .TRUE., F = .FALSE.).

## SUBROUTINE QIKGAM

*Purpose:* Generation of the 4-momentum  $q$  of the virtual photon, with the constraint  $-q^2 = Sx_{Bj}y_{Bj} \equiv Q^2 > 0$ .

*Non-local variables (re)set:*

QIPGAM (I): I-th component of the 4-momentum of the virtual photon,  $q = (q_x, q_y, q_z, q_t)$ , where  $I=\{1, 2, 3\} \Leftrightarrow \{x, y, z\}$  and  $I=4 \Leftrightarrow t$ .

*Procedure:*

With the convention  $e = (0, 0, e_z, e_t)$ ,  $e_z > 0$ , for the incoming lepton momentum in the laboratory frame and assuming  $e^2 = 0$ , the 4-momentum of the virtual photon is expressed as

$$q_x = -\sqrt{Sx_{Bj}y_{Bj}(1 - y_{Bj})} \cos \phi_q, \quad (48)$$

$$q_y = -\sqrt{Sx_{Bj}y_{Bj}(1 - y_{Bj})} \sin \phi_q, \quad (49)$$

$$q_z = y_{Bj} e_t + \frac{Sx_{Bj}y_{Bj}}{4 e_t}, \quad (50)$$

$$q_t = y_{Bj} e_t - \frac{Sx_{Bj}y_{Bj}}{4 e_t}, \quad (51)$$

according to a Sudakov decomposition. The azimuthal angle  $\phi_q$ ,  $-\pi \leq \phi_q \leq +\pi$ , is randomly generated for the default setting of the control flag QI-CONT(20) = .TRUE.. Otherwise,  $\phi_q$  is fixed at zero, i.e.  $e'$  (the 4-momentum of the scattered  $e^\pm$ ) and  $q$  are lying in the  $x - z$  plane.

## SUBROUTINE QIKGSP

*Purpose:* Generation of the 4-momenta  $q'$  and  $k$  of the virtual quark and the outgoing, on-shell current quark, respectively (c.f. Fig. 1). Implementation of the constraints  $-q'^2 = Q'^2 > 0$ , where  $Q'^2$  is the virtuality generated in QIHINS, and  $k^2 = m_k^2$ .

*Non-local variables (re)set:*

QIQGAM (I, 2): I-th component of the 4-momentum of the virtual quark,  $q' = (q'_x, q'_y, q'_z, q'_t)$ , where  $I=\{1, 2, 3\} \Leftrightarrow \{x, y, z\}$  and  $I=4 \Leftrightarrow t$ .

QIQGAM (I, 1): I-th component of the 4-momentum of the current quark,  $k = (k_x, k_y, k_z, k_t)$ , where  $I=\{1, 2, 3\} \Leftrightarrow \{x, y, z\}$  and  $I=4 \Leftrightarrow t$ .

QIWARF(12): = .FALSE. (default); reset to .TRUE. if the discriminant  $D^2 < 0$  in Eq. (57).

QINWAR(12): = 0 (default); counts the number of recurring  
 QIWARF(12) = .TRUE. settings.

*Procedure:*

By convention, the laboratory frame corresponds to the incoming proton and the incoming lepton travelling in  $-z$  and  $+z$  direction, respectively. Using a Sudakov decomposition to incorporate the required constraints on  $q'^2$  and  $k^2$ ,

$$-q'^2 = Q'^2 > 0 \text{ and } k^2 = m_k^2, \quad (52)$$

the 4-momentum  $q'$  of the virtual quark is expressed as

$$q'_x = D \cos \phi_{q'} - \frac{Q'^2}{Sx'z y_{Bj}} \sqrt{Sx_{Bj} y_{Bj} (1 - y_{Bj})} \cos \phi_q, \quad (53)$$

$$q'_y = D \sin \phi_{q'} - \frac{Q'^2}{Sx'z y_{Bj}} \sqrt{Sx_{Bj} y_{Bj} (1 - y_{Bj})} \sin \phi_q, \quad (54)$$

$$q'_z = 2 D (\cos \phi_{q'} \cos \phi_q + \sin \phi_{q'} \sin \phi_q) \sqrt{Sx_{Bj} y_{Bj} (1 - y_{Bj})} \frac{P_t}{Sy_{Bj}} \quad (55)$$

$$+ e_t \frac{Q'^2}{Sx'z} - P_t \left( \frac{Q'^2}{Sx'z y_{Bj}} (x_{Bj} - x'z + x_{Bj}(1 - y_{Bj})) - x_{Bj} - \frac{m_k^2}{Sy_{Bj}} \right),$$

$$q'_t = -2 D (\cos \phi_{q'} \cos \phi_q + \sin \phi_{q'} \sin \phi_q) \sqrt{Sx_{Bj} y_{Bj} (1 - y_{Bj})} \frac{P_t}{Sy_{Bj}} \quad (56)$$

$$+ e_t \frac{Q'^2}{Sx'z} + P_t \left( \frac{Q'^2}{Sx'z y_{Bj}} (x_{Bj} - x'z + x_{Bj}(1 - y_{Bj})) - x_{Bj} - \frac{m_k^2}{Sy_{Bj}} \right),$$

with

$$D = \sqrt{Sx_{Bj} y_{Bj} \frac{Q'^2}{Sx'z y_{Bj}} \left( \frac{Q'^2}{Sx'z y_{Bj}} - 1 \right) - Q'^2 \left( \frac{Q'^2}{Sx'z y_{Bj}} - 1 \right) - \frac{Q'^2}{Sx'z y_{Bj}} m_k^2}. \quad (57)$$

The azimuthal angle  $\phi_{q'}$ ,  $-\pi \leq \phi_{q'} \leq +\pi$ , is generated randomly. The 4-momentum of the current quark is then calculated via

$$k = q - q', \quad (58)$$

where the photon 4-momentum  $q$  has been generated in **QIKGAM**.

#### SUBROUTINE **QIKPAR**

*Purpose:* Calculation of the 4-momentum  $g$  of the incoming gluon from its generated fractional momentum  $z$  and the 4-momentum  $P$  of the

incoming proton.

*Non-local variables (re)set:*

QIPPAR (I): I-th component of the 4-momentum of the incoming gluon,  $g = (g_x, g_y, g_z, g_t)$ , where  $I = \{1, 2, 3\} \Leftrightarrow \{x, y, z\}$  and  $I = 4 \Leftrightarrow t$ .

QIPPAR (5):  $m_g$ ; HERWIG [8] mass of the incoming gluon.

*Procedure:*

The momentum vector  $g$  of the incoming, on-shell gluon (with effective (HERWIG) mass  $\sqrt{g^2} = m_g$ ) is calculated in the laboratory frame according to

$$g \equiv (g_x, g_y, g_z, g_t) = \frac{1}{2} \left( 0, 0, z(P_t + |P_z|) - \frac{m_g^2}{z(P_t + |P_z|)}, z(P_t + |P_z|) + \frac{m_g^2}{z(P_t + |P_z|)} \right), \quad (59)$$

where  $z$  denotes the generated fractional momentum of the incoming gluon and  $P = (0, 0, P_z, P_t)$  is the 4-momentum of the incoming proton. If  $P_z \leq 0$ , the sign of  $g_z$  is reversed,  $g_z \rightarrow -g_z$ .

#### SUBROUTINE **QIPLST**

*Purpose:* Assignment of masses for the  $2n_f - 1 + n_g$  outgoing partons from the instanton-induced subprocess.

*Non-local variables (re)set:*

QIPHEP (5, J): mass of the J-th outgoing parton from the instanton-induced subprocess.

QINHEP:  $2n_f - 1 + n_g$ ; number of outgoing partons from instanton subprocess.

*Procedure:*

To each outgoing parton an appropriate mass (default HERWIG [8] mass for quarks/anti-quarks, default gluon mass from **QIINIT**) is assigned.

#### SUBROUTINE **QIPSGN**

*Purpose:* Generation of the 4-momenta for the outgoing partons from the instanton-induced subprocess.

*Non-local variables (re)set:*

QIPHEP (I, J): I-th component of the 4-momentum corresponding to the J-th outgoing parton from the instanton subprocess. Here,  $I = \{1, 2, 3\} \Leftrightarrow \{x, y, z\}$  and  $I = 4 \Leftrightarrow t$ .

*Procedure:*

- By means of the MAMBO [26] algorithm<sup>5</sup>, the momenta  $p_j$  of the  $n = 2n_f - 1 + n_g$  outgoing partons in the  $q'g$  CMS are generated *uniformly* in phase space,

$$\int \prod_{j=1}^n \left\{ d^4 p_j \delta^{(+)}(p_j^2 - m_j^2) \right\} \delta^{(3)}\left(\sum_{k=1}^n \vec{p}_k\right) \delta\left(W_I - \sum_{k=1}^n p_k^t\right). \quad (60)$$

The masses  $m_j$  were assigned in the subroutine **QIPLST**.

- Next, for the default setting of the control flags in **QIINIT** (QICONT(1) = .TRUE. in Table 5), different energy weights for gluons and quarks (**QIP-SWT**) are implemented by means of the rejection method. The resulting momenta  $p_j$  are then *uniformly distributed in energy-weighted phase space*, Eq. (10), corresponding to the leading-order matrix elements [3].

## SUBROUTINE **QIPSTO**

*Purpose:* Store 4-momenta and particle identity codes of all outgoing partons in the PHEP common block of HERWIG [8] and set appropriate IHEP pointers.

*Non-local variables (re)set:*

PHEP (I, IHEP):	I-th 4-momentum component of the J-th outgoing parton from the instanton subprocess, with IHEP=10+J and $1 \leq J \leq 2n_f - 1 + n_g$ .
IDHEP (IHEP):	particle data group [16] identity code (ID-PDG) of the J-th outgoing parton.
IDHW (IHEP):	HERWIG identity code of J-th outgoing parton.
QIPLIS (JLP, ILP):	IHEP pointer referring to the outgoing parton JLP in the string ILP.

*Remarks:* See also the descriptions of the routines **QISTID** and **QIGLST**.

## SUBROUTINE **QIPSWT** (PSWGT)

*Purpose:* Calculation of the relative energy-weight factor (c.f. Eq. (10)) for the generated momenta of the outgoing partons, as corresponding to the modulus squared of the leading-order matrix elements.

*Argument:* PSWGT: relative energy weight (63).

*Procedure:*

---

<sup>5</sup> The MAMBO algorithm implemented in the Monte Carlo generator for baryon number violating interactions HERBVI [23] is actually used and provided in the source file 'saddle.F' of the QCDINS distribution.

An energy-weight factor  $w$  corresponding to the modulus squared of the leading-order matrix elements [3] is calculated as follows<sup>6</sup>: Each outgoing quark with four-momentum  $p_q$  is weighted by its energy  $p_q^t$ , each outgoing gluon with four-momentum  $p_k$  by its energy squared  $p_k^{t2}$ , such that

$$w = \prod_{q=1}^{2n_f-1} p_q^t \prod_{k=1}^{n_g} p_k^{t2}. \quad (61)$$

It is easy to show that the corresponding maximum weight is given by

$$w_{\max} = 2^{2n_g} \left[ \frac{W_I}{2(n_g + n_f) - 1} \right]^{2(n_g + n_f) - 1}. \quad (62)$$

The subroutine **QIPSWT** returns the relative weight

$$w_{\text{rel}} = w/w_{\max} \quad (63)$$

in the variable PSWGT.

SUBROUTINE **QIPVWT** (WT)

*Purpose:* Calculation of the remaining weight factors required for a properly normalized cross section (3).

*Argument:* WT: returned weight factor (64).

*Procedure:*

The weight factor

$$W_n = 2\pi\alpha^2 x_{\text{Bj}} x' \sum_{q'=d,u,s,\dots;\bar{d},\bar{u},\bar{s},\dots} e_{q'}^2 \quad (64)$$

is calculated. Here,  $\alpha$  is the electro-magnetic fine-structure constant and  $e_{q'}$  denotes the fractional electro-magnetic charge of the virtual (anti-)quark  $q'$ . The sum extends over quarks and anti-quarks of the considered  $n_f$  light flavours.

SUBROUTINE **QIRDIS** (LU, LL, X, WGT, N)

*Purpose:* Strong increase of efficiency through generation of  $X = Q'^2, x'$  as  $dX/X^{N+1}$ .

*Arguments:*

---

<sup>6</sup> We thank M. Seymour for pointing out an error in the previous version of this subroutine and for providing us with a corrected version [27] of it.

- LU: logarithm of upper integration limit  $X_U$  in Eq. (65).
- LL: logarithm of lower integration limit  $X_L$  in Eq. (65).
- N: power in Eq. (66).
- X:  $X$  value associated with the uniformly distributed  $Z$  according to Eq. (66).
- WGT: Monte Carlo weight (67) with  $f \equiv 1$ .

*Remarks:* The instanton-induced cross section (3) involves integrations

$$I(X_U, X_L) = \int_{X_L}^{X_U} \frac{dX}{X} f(X), \quad (65)$$

where, typically, the function  $f(X)$  *grows steeply towards small  $X$* . This makes the *standard* Monte Carlo evaluation (e. g. Eqs. (31), (32)) of the integral (65) very inefficient.

*Procedure:*

The efficiency is strongly increased by means of the present routine. First, the integration variable is changed to

$$Z = X^{-N}; \quad dZ = -N X^{-(N+1)} dX, \quad (66)$$

with the power  $N$  empirically optimized and typically ranging between 2.5 and 5.0. Uniformly distributed random points  $Z = X^{-N}$  are then generated in the interval  $X_U^{-N} \leq Z \leq X_L^{-N}$ . With this procedure, the weight corresponding to the integral (65) takes the form

$$W = \frac{1}{N} (X_L^{-N} - X_U^{-N}) \frac{f(X = Z^{-1/N})}{Z}. \quad (67)$$

SUBROUTINE **QISETD** (NUM, VALUE, OK)

*Purpose:* Set double precision parameter QIUPAR(NUM) to a desired value.

*Arguments:*

- NUM: integer, pointing to the parameter QIUPAR(NUM) to be changed.
- VALUE: desired double precision value of QIUPAR(NUM).
- OK: logical return flag.

*Non-local variables (re)set:*

- QINWAR(9): = QINWAR(9)+1; counts attempts to (re)set non-existing parameter QIUPAR(.).
- QIWARF(9): = .TRUE. if parameter index NUM out of range.
- QIRCAL: = .TRUE. if QIWARF(9) = .FALSE. (default).

*Remarks:* Service routine for resetting the default double precision input parameters QIUPAR(NUM), NUM=1,2,...,18, set in **QIINIT** as in Table 4, to the desired value VALUE. On return, the logical flag OK is .TRUE. if NUM is within its allowed range.

SUBROUTINE **QISETF** (NUM, FLAG, OK)

*Purpose:* Set logical flag QICONT(NUM) to a desired value.

*Arguments:*

NUM: integer, pointing to the parameter QICONT(NUM) to be changed.  
 FLAG: desired boolean value of QICONT(NUM).  
 OK: logical return flag.

*Non-local variables (re)set:*

QINWAR(5): = QINWAR(5)+1; counts attempts to (re)set non-existing parameter QICONT(.).  
 QIWARF(5): = .TRUE. if parameter index NUM out of range.  
 QIRCAL: = .TRUE. if QIWARF(5) = .FALSE. (default).

*Remarks:* Service routine for resetting the default boolean input parameters QICONT(NUM), NUM=1,2,...,21, set in **QIINIT** as in Table 5, to the desired value FLAG. On return, the logical flag OK is .TRUE. if NUM is within its allowed range.

SUBROUTINE **QISETI** (NUM, VALUE, OK)

*Purpose:* Set integer parameter QIPARI(NUM) to a desired value.

*Arguments:*

NUM: integer, pointing to the parameter QIPARI(NUM) to be changed.  
 VALUE: desired integer value of QIPARI(NUM).  
 OK: logical return flag.

*Non-local variables (re)set:*

QINWAR(7): = QINWAR(7)+1; counts attempts to (re)set non-existing parameter QIPARI(.).  
 QIWARF(7): = .TRUE. if parameter index NUM out of range.  
 QIRCAL: = .TRUE. if QIWARF(7) = .FALSE. (default).

*Remarks:* Service routine for resetting the default integer input parameters QIPARI(NUM), NUM=1,2,...,10, set in **QIINIT** as in Table 4, to the desired value VALUE. On return, the logical flag OK is .TRUE. if NUM is within its allowed range.



## SUBROUTINE **QISPLT** (WEIGHT)

*Purpose:* Calculation of the weight associated with the flux of the virtual (anti-)quark  $q'$  from the  $\gamma^* q' k$  vertex (c.f. Fig. 1).

*Argument:* WEIGHT: returned weight factor (68).

*Procedure:*

The weight

$$W_{q'} = \frac{1}{x'z} P_{q'}^{(I)} \quad (68)$$

is calculated, where  $P_{q'}^{(I)}$  is the flux factor (4) from Refs. [4,14].

## SUBROUTINE **QISTAT**

*Purpose:* Print input parameter vectors QIUPAR, QIPARI and QICONT, as well as possible warnings (QIWARF). For default values, see Tables 4 and 5.

## SUBROUTINE **QISTID**

*Purpose:* Generation of identity codes, 4-momenta and colour/flavour connections of the  $2n_f - 1 + n_g$  outgoing partons of the instanton-induced subprocess  $g + q' \xrightarrow{I} (2n_f - 1) \cdot q + n_g \cdot g$ .

*Procedure:*

- Given are the identity codes of the incoming partons, the number  $n_g + 1$  of gluons and the required “flavour democracy” of the possible partonic subprocesses like e.g. for  $n_f = 3$  and  $n_g = 4$ ,

$$s + g \xrightarrow{I} d + \bar{d} + u + \bar{u} + s + 4 \cdot g. \quad (69)$$

The structure as well as the identity codes of the partonic final state are then set up by the following two steps:

- First,  $n_f [q \dots \bar{q}]$  - “strings” of partons are generated (**QIGLST**). Each begins with a quark, followed by a random number  $\leq n_g + 1$  of gluons, and ends with an anti-quark of randomly chosen flavour. Due to flavour democracy,  $q\bar{q}$ -pairs of all  $n_f$  flavours must occur precisely once, e.g. for the process (69) above,

$$[d \, g \, g \, \bar{s}] \quad [u \, g \, \bar{d}] \quad [s \, g \, g \, \bar{u}]. \quad (70)$$

All partons are marked as outgoing at this stage.

- Next (**QIGPAR**), one of the  $n_g + 1$  gluons in the above strings is randomly marked as incoming. Furthermore, the anti-parton corresponding to the virtual (anti-)quark  $q'$  is identified and marked as incoming, e. g. ( $\bullet$ ) for the process (69) and string configuration (70) above,

$$[d \ g \ g \ \overset{\bullet}{\bar{s}}] \quad [u \ g \ \bar{d}] \quad [s \ g \ \overset{\bullet}{g} \ \bar{u}]. \quad (71)$$

- The assignment of the final state parton momenta is based on the crucial requirement of isotropy in the “instanton rest frame”,  $\vec{q}' + \vec{g} = \vec{0}$ . It proceeds through the following steps:
  - The appropriate (HERWIG [8]) mass  $m_i$  is assigned to each of the  $2n_f - 1 + n_g$  outgoing partons  $i$  (**QIPLST**).
  - The 4-momenta  $p_i$  in the instanton rest frame are generated uniformly in energy-weighted phase-space (10), corresponding to the leading-order matrix element [3] with different energy weights for gluons and quarks (**QIPSGN**).
  - The four-momenta and particle identity codes of all outgoing partons are stored in the PHEP common block of HERWIG (**QIPSTO**). The corresponding IHEP pointers start at IHEP=11 for the first outgoing parton from the instanton subprocess (a  $d$  quark in our example (71) above) and are increased consecutively along the strings, e. g. for the process (69) and string configuration (71) above, the IHEP pointers would read

$$\begin{array}{ccc} [d & g & g \ \overset{\bullet}{\bar{s}}] & [u & g \ \bar{d}] & [s & g \ \overset{\bullet}{g} \ \bar{u}] \\ 11 & 12 & 13 & 14 & 15 & 16 & 17 & 18 & 19 \end{array} .$$

- Finally (**QICCON**), the stored list of IHEP pointers is augmented by those of the current quark (IHEP=10) and of the incoming gluon (IHEP=6), as assigned in **QIHGEN**. For the example above, this means

$$\begin{array}{ccc} [d & g & g \ \overset{\bullet}{\bar{s}}] & [u & g \ \bar{d}] & [s & g \ \overset{\bullet}{g} \ \bar{u}] \\ 11 & 12 & 13 & \mathbf{10} & 14 & 15 & 16 & 17 & 18 & \mathbf{6} & 19 \end{array} .$$

As a main issue, the colour/flavour connections are established in **QICCON** as follows: The colour flow is constructed by connecting the colour lines of neighbouring partons within each of the strings. The flavour flow is constructed by connecting the flavour lines of the quark at the beginning of a string with the flavour line of the anti-quark at the end of a string. For

IHEP	Description	JMOHEP(2,IHEP)	JDAHEP(2,IHEP)
11	$d$ out	12	10
12	$g$ out	13	11
13	$g$ out	10	12
10	$\bar{s}$ out (current quark)	11	13
14	$u$ out	15	16
15	$g$ out	16	14
16	$\bar{d}$ out	14	15
17	$s$ out	18	19
18	$g$ out	6	17
6	$g$ in	19	18
19	$\bar{u}$ out	17	6

Table 6

HERWIG [8] mother/daughter pointers specifying the colour/flavour flow for the example (69) in the description of subroutine **QISTID**.

the example above, the corresponding HERWIG mother/daughter pointers specifying the colour/flavour flow are then as in Table 6.

#### SUBROUTINE **QIUSPS (WT)**

*Purpose:* Dummy routine for optional modification of relative phase space weight as calculated in **QIPSWT**.

*Arguments:* WT: modified relative phase space weight.

*Remarks:* Called from **QIPSWT** if QICONT(2) = .FALSE.. Calculation of WT has to be provided by the user.

#### FUNCTION **XI** (XPR, XI\_MIN, XI\_MAX, XQ, XMU, NF, LOOPFL)

*Purpose:* The saddle point value of the conformally invariant  $I\bar{I}$ -separation  $\xi$  is calculated as function of  $x'$ ,  $4\pi/\alpha_{\overline{\text{MS}}}(Q')$ ,  $4\pi/\alpha_{\overline{\text{MS}}}(\mu_r)$  and  $n_f$ .

*Arguments:*

XPR:  $x'$

XI\_MIN:  $\xi_{\min}$ ; lower boundary of  $\xi$  used for interpolation.

XI\_MAX:  $\xi_{\max}$ ; upper boundary of  $\xi$  used for interpolation.

XQ:  $4\pi/\alpha_{\overline{\text{MS}}}(Q')$

XMU:  $4\pi/\alpha_{\overline{\text{MS}}}(\mu_r)$

NF:  $n_f$ ; number of light flavours.

LOOPFL: = 1: 1-loop renormalization group (RG) invariance [4]  
along with 1-loop form of  $\alpha_s$ .

- = 2: 2-loop RG invariance [4] along with 2-loop form of  $\alpha_{\overline{\text{MS}}}$ .
- = 3: (default) 2-loop RG invariance along with 3-loop form of  $\alpha_{\overline{\text{MS}}}$ .

*Procedure:*

First, the saddle point equation (18) is solved analytically for  $x'$ , and the  $x'_i$ -values corresponding to a discrete set of  $\xi_i$  values are calculated as

$$x'_i = \frac{(\xi_i - 2)}{(\xi_i + 2) + 4\tilde{S}(\xi_i)(\tilde{S}(\xi_i) - 2v_i)/v_i^2}, \quad (72)$$

with  $\xi_{\min} \leq \xi_i \leq \xi_{\max}$  and  $v_i$  from Eqs. (19)–(22) inserted:

$$v_i = v_i(\xi_i, X(Q'), X(\mu_r)) = 2 D(\tilde{S}) \times \quad (73)$$

$$W \left( \frac{\exp \left\{ \frac{1}{2} \frac{\tilde{S}}{D(\tilde{S})} + \frac{1}{2} \frac{\Delta_1 - 1}{\Delta_1 \beta_0} \left[ \Delta_1 \ln \left( \frac{\Delta_1 X(\mu_r)}{X(Q') + (\Delta_1 - 1) X(\mu_r)} \right) - 1 \right] X(\mu_r) + \frac{1}{2} \frac{X(Q')}{\beta_0} \right\}}{2 D(\tilde{S})} \right).$$

In Eq. (73), the explicit dependence of  $v_i$  on  $Q'/\mu_r$  (c.f. Eq. (19) has been eliminated in favour of an  $X(Q')$ ,  $X(\mu_r)$  dependence by means of the standard scale transformation of  $\alpha_{\overline{\text{MS}}}$ . Here, we have introduced the shorthand

$$X(M) \equiv \frac{4\pi}{\alpha_{\overline{\text{MS}}}(M)}. \quad (74)$$

The desired continuous inversion  $\xi_* = \xi_*(x', \dots)$  is then achieved by means of numerical interpolation based on the above exact supporting points  $(\xi_i, x'_i)$ .

**FUNCTION XQS (QLAM, LOOPFL, NF)**

*Purpose:* Calculation of  $4\pi/\alpha_{\overline{\text{MS}}}$  as function of  $M/\Lambda_{\overline{\text{MS}}}^{(n_f)}$ , where  $M$  is a generic mass scale.

*Arguments:*

- QLAM:  $M/\Lambda_{\overline{\text{MS}}}^{(n_f)}$
- LOOPFL: = 1: 1-loop form of  $\alpha_s$ .  
 = 2: 2-loop form of  $\alpha_{\overline{\text{MS}}}$ .  
 = 3: (default) 3-loop form of  $\alpha_{\overline{\text{MS}}}$ .
- NF:  $n_f$ ; number of light flavours.

*Procedure:*

The running coupling  $\alpha_{\overline{\text{MS}}}$  is calculated according to the explicit formula Eq. (9.5a) in Ref. [16], which is accurate to 3-loop. The quantity  $4\pi/\alpha_{\overline{\text{MS}}}$  is returned. The integer variable `LOOPFL` = 1, 2, 3 controls the loop-order at which Eq. (9.5a) in Ref. [16] is truncated.

## 4 Usage and availabiliy

QCDINS 2.0 should be loaded together with HERWIG [8] version 5.9 and JETSET [18] version 7.4, that are part of the CERNLIB distribution. The program is a slave system, which the user must call from his own steering program. A very simple example is provided in Appendix A. By default, QCDINS is compiled in form of a library, 'libqcdins.a', that may be linked together with 'libherwig59.a', 'libjetset74.a' and the library 'libpdfplib.a' of parton distribution functions to the steering program. An extensive demonstration program, including an interface to the HZTOOL [28] package, and a detailed installation instruction are included in the distribution.

Information about the distribution, its update history, an interactive manual, the source code, pictures of typical events etc. can be accessed via the QCDINS WWW site, <http://www.desy.de/~t00fri/qcdins/qcdins.html>.

## Acknowledgements

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## Appendix A: Simple steering program

The following code may serve as the simplest illustration of a steering program for the QCDINS/HERWIG package. Note that the two subroutines

**HWANAL** and **HWAEND** must exist.

For an example of an interface with the JETSET hadronization, we refer to the extensive steering program 'qtesthz' included in the QCDINS distribution.

```
PROGRAM QCDINS
#include "herwig.inc"
C Force inclusion of block data
EXTERNAL HWUDAT

C Initialize process number
IPROC = 17600
C Maximal number of events in this run
MAXEV = 1000
C Beam particles
PBEAM1 = 27.5D0
PBEAM2 = 820.0D0
PART1 = 'E+'
PART2 = 'P'
C Initialize common blocks
CALL HWIGIN
C User can reset parameters at this point, otherwise values
C set in HWIGIN will be used.
C No vertex information in event printout
PRVTX=.FALSE.
C Reset number of shots for initial max weight search
IBSH = 5000
LRSUD=0
LWSUD=77
C Seeds
NRN(1)=106645412
NRN(2)=135135176
C Use laboratory frame
USECMF = .FALSE.
C Compute parameter-dependent constants
CALL HWUINC
C Number of HERWIG events to print out
MAXPR = 1
C Call hwusta to make any particle stable
CALL HWUSTA('PIO  ')
CALL HWUSTA('K_SO  ')

C Initialize default QCDINS input parameters
CALL QIINIT
C Print input parameters
CALL QISTAT
C Loop over events
CALL QCLOOP

C User's terminal calculations
CALL HWAEND
STOP
END

SUBROUTINE HWANAL
RETURN
END

SUBROUTINE HWAEND
RETURN
END
```

## Appendix B: Test run output

Below, we display the essential output from a test run of the very simple steering program from Appendix A. This test run simulates 1000 complete instanton-induced events in deep-inelastic  $e^+P$  scattering (HERA), with  $E_{e^+} = 27.5$  GeV and  $E_P = 820$  GeV, in the laboratory frame. All the QCDINS parameters correspond to the default values as set in the initialization routine **QIINIT** (c.f. Tables 4 and 5).

For reasons of space, the display of the first event has been truncated after the hard subprocess level.

```

...
...

INPUT CONDITIONS FOR THIS RUN

BEAM 1 (E+      ) MOM. =    27.50
BEAM 2 (P       ) MOM. =   820.00
PROCESS CODE (IPROC) =   17600

...
...

=====
QCD Instanton Monte Carlo Information          Version 2.0
=====
Parameter                                     Value
=====
Default gluon mass (GeV)                     0.7500E+00
Minimum allowed value of x_bj                 0.1000E-02
Maximum allowed value of z (proton mom.frac.) 0.1000E+01
Maximum allowed value of y_bj                 0.1000E+01
Minimum allowed value of y_bj                 0.1000E+00
Maximum allowed value of x prime               0.9000E+00
Minimum allowed value of x prime               0.3500E+00
Maximum allowed value of Q prime **2 (GeV**2) 0.1652E+04
Minimum allowed value of Q prime **2 (GeV**2) 0.1134E+03
Lower cut for ME calculation on x prime        0.3500E+00
Lowest allowed weight efficiency cut           -.1000E-09
Minimum instanton invariant mass               0.0000E+00
Lambda-MS-bar(nf) [GeV] from PDG 1998        0.3459E+00
Minimum total K.E. of outgoing partons (GeV)  0.0000E+00
Renormalization point KAPPA = mu_r/Qprime:    0.1500E+00
Minimum allowed value of Q **2 (GeV**2)        0.1134E+03
Factorization scale (GeV)                     0.1065E+02
=====
ID code assumed for instanton                  206
Maximum number of MAMBO iterations per PS wt. 100
Maximum number of PS wt. rejections per event 300
Number nf of (light) flavours                  3
Maximum average gluon multiplicity in distbn. 10
Maximum number of iterations for ME generation 20
Maximum number of QIGMUL iterations            40
Number of loops in RG-invariance/alpha_s       3
=====

```

Control flag option	Setting
Reweight phase space configurations	True
Use default phase space reweighting	True
Use Matrix element weight	True
Disregard instanton minimum mass requirement	True
Generate Q prime before x prime	True
Enforce mass of current quark in kinematics	True
Enforce limit on maximum number of gluons	True
Ensure mass less than subprocess energy	True
Kill events with insufficient instanton mass	True
Use z generation as dz/z	True
Use x prime **n generation for efficiency	True
Use Q prime **n generation for efficiency	True
Use HERWIG rather than JETSET hadronization	True
Use random azimuth angle for scattered electron	True
Use full hadronization	True

#### INITIAL SEARCH FOR MAX WEIGHT

```

PROCESS CODE IPROC =      17600
RANDOM NO. SEED 1   =      1246579
                SEED 2   =      8447766
NUMBER OF SHOTS    =      5000

```

```

*****
*                               *
*   QCDINS version 2.0         *
*                               *
*****

```

...

...

```

NEW MAXIMUM WEIGHT = 2.4520378923431534E-05
NEW MAXIMUM WEIGHT = 6.0858601240747906E-02
NEW MAXIMUM WEIGHT = 0.1289870599803515
NEW MAXIMUM WEIGHT = 0.3662942637479250
NEW MAXIMUM WEIGHT = 0.5705336816482935
NEW MAXIMUM WEIGHT = 0.8061467165013312

```

INITIAL SEARCH FINISHED

OUTPUT ON ELEMENTARY PROCESS

```

NUMBER OF EVENTS   =      0
NUMBER OF WEIGHTS  =     5000
MEAN VALUE OF WGT  = 2.8721E-02
RMS SPREAD IN WGT  = 6.4377E-02
ACTUAL MAX WEIGHT  = 7.3286E-01
ASSUMED MAX WEIGHT = 8.0615E-01

```

```

PROCESS CODE IPROC =      17600
CROSS SECTION (PB) =    28.72
ERROR IN C-S (PB)  =    0.9104
EFFICIENCY PERCENT =    3.563

```

EVENT        1:    27.50 GEV/C E+            ON 820.00 GEV/C P            PROCESS: 17600

SEEDS: 106645412 & 135135176    STATUS: 100    ERROR:    0    WEIGHT: 0.2872E-01



---INITIAL STATE---

IHEP	ID	IDPDG	IST	MO1	MO2	DA1	DA2	P-X	P-Y	P-Z	ENERGY	MASS
1	E+	-11	101	0	0	4	0	0.00	0.00	27.50	27.50	0.00
2	P	2212	102	0	0	0	0	0.00	0.00	-820.00	820.00	0.94
3	CMF	0	103	1	2	0	0	0.00	0.00	-792.50	847.50	300.33

---INITIAL STATE---

IHEP	ID	IDPDG	IST	MO1	MO2	DA1	DA2	P-X	P-Y	P-Z	ENERGY	MASS
4	E+	-11	101	1	0	0	0	0.00	0.00	27.50	27.50	0.00

---HARD SUBPROCESS---

IHEP	ID	IDPDG	IST	MO1	MO2	DA1	DA2	P-X	P-Y	P-Z	ENERGY	MASS
5	E+	-11	121	7	9	21	9	0.00	0.00	27.50	27.50	0.00
6	GLUON	21	122	7	20	22	19	0.00	0.00	-50.37	50.38	0.75
7	HARD	0	120	5	6	9	20	0.53	0.99	-22.98	77.98	74.51
8	INST	0	3	7	0	0	0	0.23	9.33	-43.54	47.01	15.07
9	E+	-11	123	7	5	26	5	8.20	-7.47	3.48	11.63	0.00
10	UBAR	-2	124	7	14	27	17	-8.43	-1.86	17.19	19.24	0.31
11	DQRK	1	124	7	12	31	13	-0.07	0.52	-7.65	7.67	0.32
12	GLUON	21	124	7	13	33	11	0.16	-0.28	-0.64	1.04	0.75
13	DBAR	-1	124	7	11	35	12	-0.67	-0.12	-2.65	2.75	0.32
14	UQRK	2	124	7	15	37	10	0.01	4.97	-11.73	12.75	0.32
15	GLUON	21	124	7	16	39	14	0.53	0.62	-2.17	2.44	0.75
16	GLUON	21	124	7	17	41	15	0.43	-0.43	-8.44	8.49	0.75
17	GLUON	21	124	7	10	43	16	-0.72	0.09	-2.40	2.62	0.75
18	SQRK	3	124	7	19	45	20	-0.11	2.50	-4.93	5.55	0.50
19	GLUON	21	124	7	6	47	18	0.81	0.93	-1.46	2.06	0.75
20	SBAR	-3	124	7	18	51	6	-0.14	0.52	-1.47	1.64	0.50
21	Z0/GAMA*	23	3	5	7	0	0	-8.20	7.47	24.02	15.87	-21.17

...

...

CHECK OF ENERGY-MOMENTUM CONSERVATION IN THE EVENT:

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Sum\_i(P\_i)[GeV] = ( 4.87E-13 -5.49E-13 1.59E-12 -4.20E-12 )

with 60 stable particles in final state contributing.

OUTPUT ON ELEMENTARY PROCESS

NUMBER OF EVENTS = 1000  
NUMBER OF WEIGHTS = 27258  
MEAN VALUE OF WGT = 2.8837E-02  
RMS SPREAD IN WGT = 6.3371E-02  
ACTUAL MAX WEIGHT = 7.0199E-01  
ASSUMED MAX WEIGHT = 8.0615E-01

PROCESS CODE IPROC = 17600  
CROSS SECTION (PB) = 28.84  
ERROR IN C-S (PB) = 0.3838  
EFFICIENCY PERCENT = 3.577

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